Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJYC1621

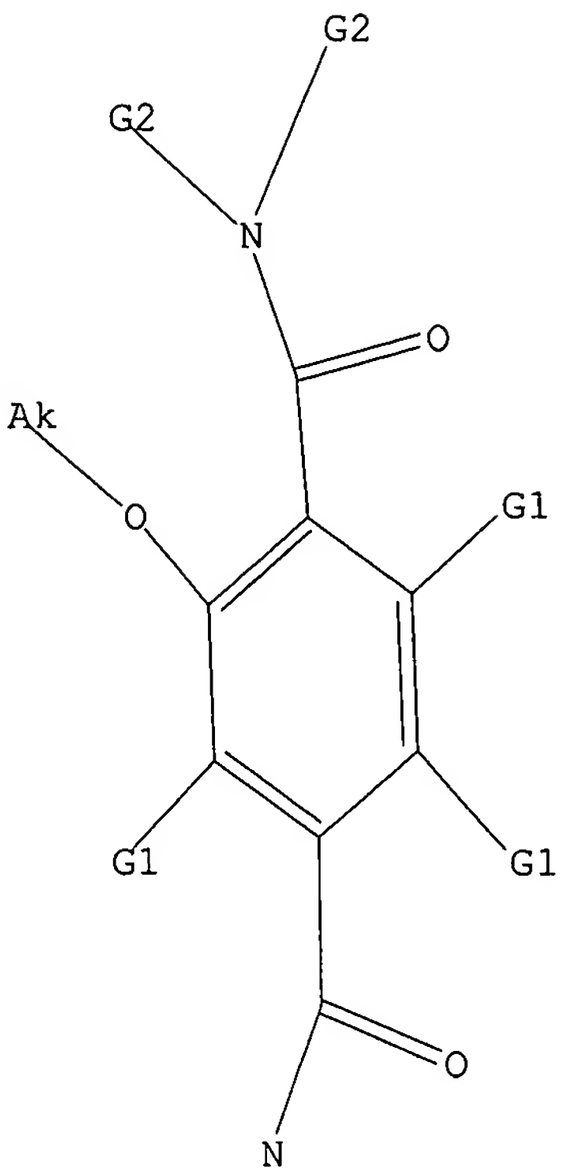
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 4	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 5	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 7	AUG 27	USPATOLD now available on STN
NEWS 8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 10	SEP 13	FORIS renamed to SOFIS
NEWS 11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 12	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 13	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS 14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 15	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 16	OCT 19	BEILSTEIN updated with new compounds
NEWS 17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS 18	NOV 19	WPIX enhanced with XML display format
NEWS 19	NOV 30	ICSD reloaded with enhancements
NEWS 20	DEC 04	LINPADOCDB now available on STN
NEWS 21	DEC 14	BEILSTEIN pricing structure to change
NEWS 22	DEC 17	USPATOLD added to additional database clusters
NEWS 23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS 24	DEC 17	DGENE now includes more than 10 million sequences
NEWS 25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS 26	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 27	DEC 17	CA/CAplus enhanced with new custom IPC display formats
NEWS 28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS 29	JAN 02	STN pricing information for 2008 now available
NEWS 30	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 31	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 32	JAN 28	MARPAT searching enhanced
NEWS 33	JAN 28	USGENE timeliness enhanced
NEWS 34	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 35	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,

```
                CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
                AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

 NEWS HOURS     STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN     Welcome Banner and News Items
 NEWS IPC8      For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN Customer
  agreement.  Please note that this agreement limits use to scientific
  research.  Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 18:19:13 ON 28 JAN 2008
=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 18:19:31 ON 28 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   27 JAN 2008  HIGHEST RN 1000849-38-6
DICTIONARY FILE UPDATES:  27 JAN 2008  HIGHEST RN 1000849-38-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\jcho2\My Documents\10588478-c.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1                STR
```



G1 C,H,S,N

G2 H,Ak,NH,NH2

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 18:19:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3389 TO ITERATE

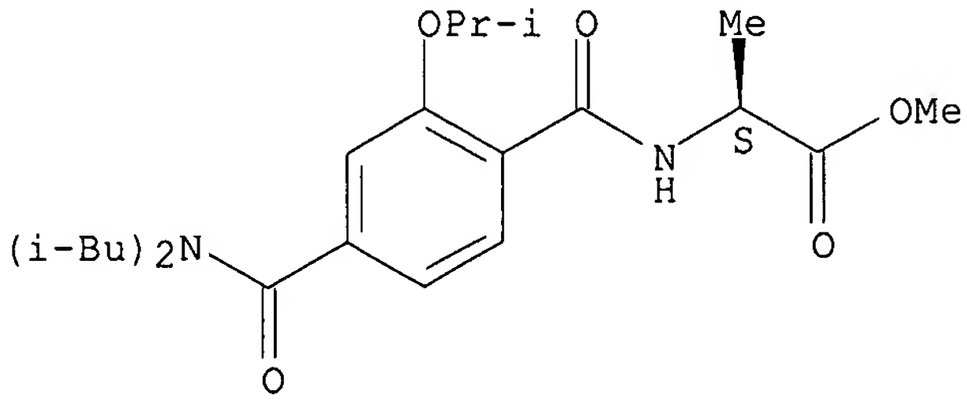
100.0% PROCESSED 3389 ITERATIONS 196 ANSWERS
SEARCH TIME: 00.00.01

L2 196 SEA SSS FUL L1

=> d scan

L2 196 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF C23 H36 N2 O5

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	178.36	178.57

FILE 'CAPLUS' ENTERED AT 18:20:09 ON 28 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 28 Jan 2008 VOL 148 ISS 5
FILE LAST UPDATED: 27 Jan 2008 (20080127/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l2
L3 28 L2

=> d l3 1-17 bib abs hitstr

L3 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:63581 CAPLUS
DN 146:156259
TI MAO-B inhibitors useful for treating obesity
IN Mcelroy, John F.; Chorvat, Robert J.; Rajagopalan, Parthasarathi
PA Jenrin Discovery, USA
SO PCT Int. Appl., 92pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007008963	A1	20070118	WO 2006-US27019	20060712

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,

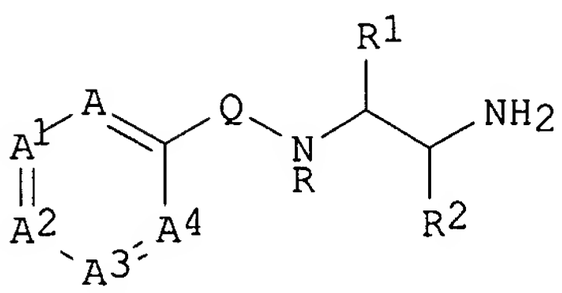
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

US 2007015734 A1 20070118 US 2006-456912 20060712

PRAI US 2005-698867P P 20050713

OS MARPAT 146:156259

GI



I

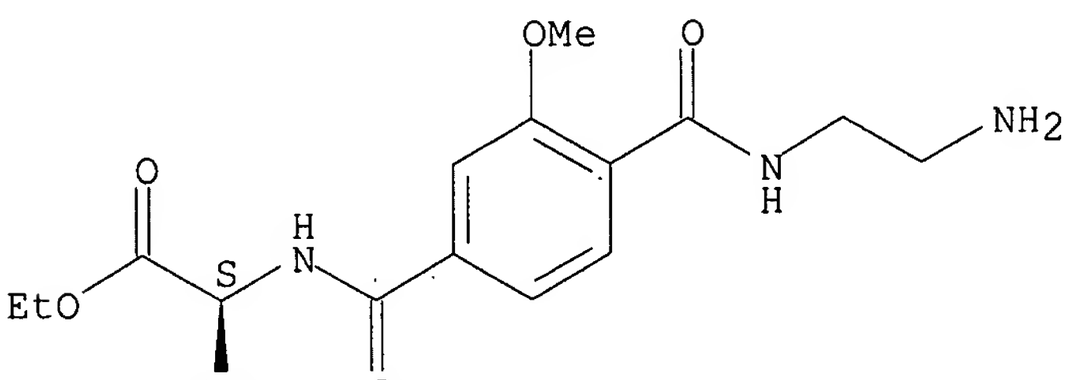
AB The invention provides novel compds. of formula I (where A, A1, A2, A3, and A4, are independently selected from CH, substituted C, N, and N+-O-, provided that from 0-1 is N+-O-; R is independently selected from H and C1-6 alkyl; R1 is selected from H and C1-6 alkyl; R2 is selected from H and C1-6-alkyl; Q is selected from C=O and SO2) that are monoamine oxidase-B (MAO-B) inhibitors, which can be useful in treating obesity, diabetes, and/or cardiometabolic disorders (e.g., hypertension, dyslipidemias, high blood pressure, and insulin resistance).

IT 919772-32-0 919772-33-1 919772-34-2
919772-35-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(MAO-B inhibitors useful for treating obesity and other disorders)

RN 919772-32-0 CAPLUS

CN L-Alanine, N-[4-[[(2-aminoethyl)amino]carbonyl]-3-methoxybenzoyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

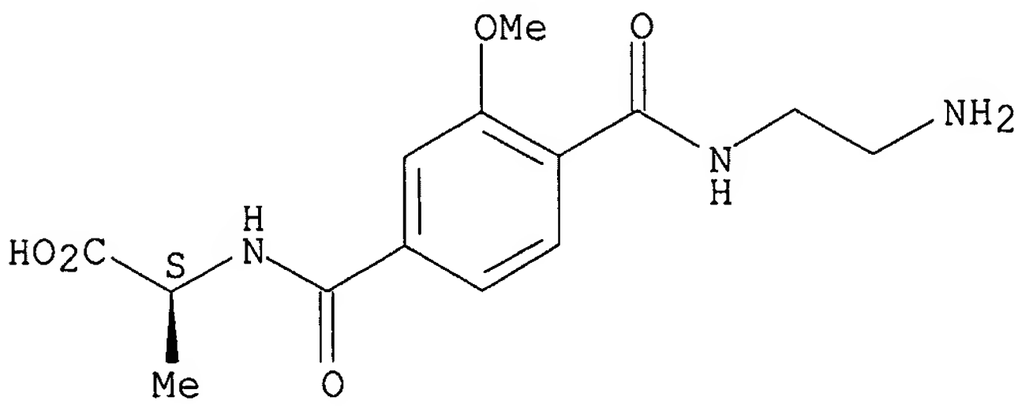


Me O

RN 919772-33-1 CAPLUS

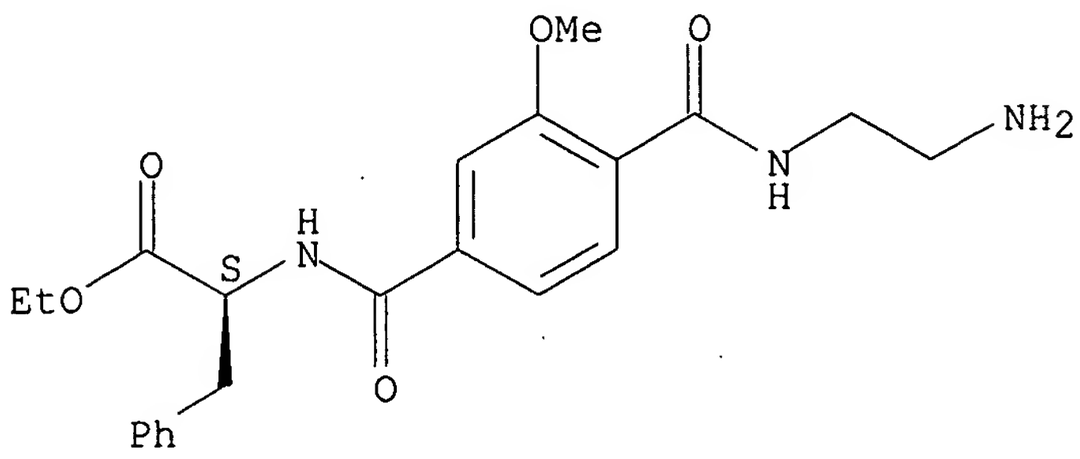
CN L-Alanine, N-[4-[[(2-aminoethyl)amino]carbonyl]-3-methoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



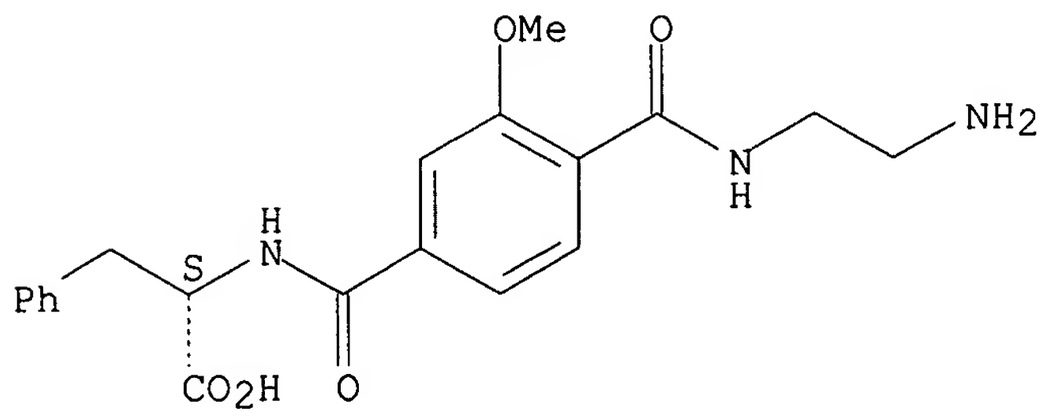
RN 919772-34-2 CAPLUS
CN L-Phenylalanine, N-[4-[[(2-aminoethyl)amino]carbonyl]-3-methoxybenzoyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 919772-35-3 CAPLUS
CN L-Phenylalanine, N-[4-[[(2-aminoethyl)amino]carbonyl]-3-methoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:656393 CAPLUS
DN 145:124546
TI Preparation of benzoxazole derivatives for the manufacture of ophthalmic lenses
IN Kauffman, Joeel; Litak, Peter T.; Rickwood, Martin
PA Essilor International (Compagnie Generale D'Optique), Fr.
SO PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006069811	A2	20060706	WO 2005-EP14202	20051230
WO 2006069811	A3	20070104		

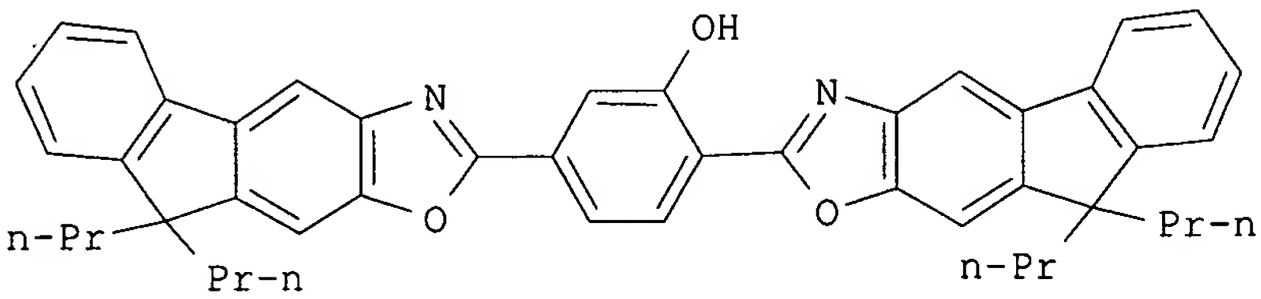
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,

GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

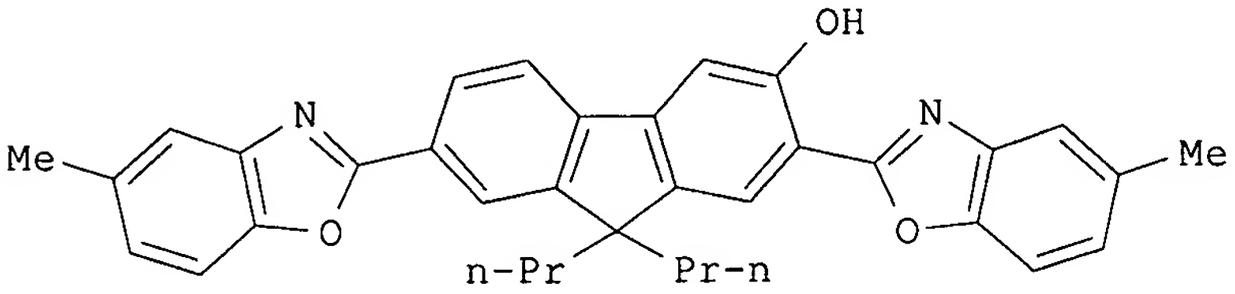
	AU 2005321406	A1	20060706	AU 2005-321406	20051230
	CA 2592585	A1	20060706	CA 2005-2592585	20051230
	EP 1838682	A2	20071003	EP 2005-850391	20051230
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRAI	US 2004-640506P	P	20041230		
	WO 2005-EP14202	W	20051230		

OS MARPAT 145:124546

GI



I



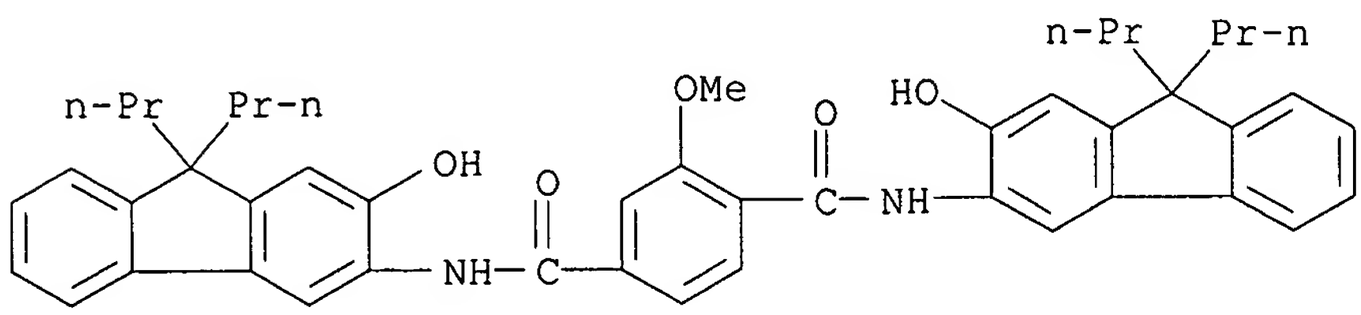
II

AB Compds. that absorb UV light 380 nm to 400 nm range but avoid absorption in the blue light range, thereby imparting yellowness, i.e., 410-420 nm have suitable refractive characteristics useful in the preparation of optical resins or plastics suitable, for example, for the manufacture of ophthalmic lenses. Methods for making the compds. I and II, which were prepared in a multi-step synthesis starting from 2-methoxyterephthalic acid and 3-methoxyfluorene resp., optic lenses containing the compds., and methods for making these are also described.

IT 897364-45-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 9H-fluoreno[3,2-d]oxazole and benzoxazolylfluorene derivs. as optical lenses)

RN 897364-45-3 CAPLUS

CN 1,4-Benzenedicarboxamide, N,N'-bis(2-hydroxy-9,9-dipropyl-9H-fluoren-3-yl)-2-methoxy- (9CI) (CA INDEX NAME)



L3 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2006:127910 CAPLUS

DN 144:378247

TI Synthesis and characterization of new electroluminescent molecules

containing carbazole and oxadiazole units

AU Bugatti, Valeria; Concilio, Simona; Iannelli, Pio; Piotto, Stefano P.; Bellone, Salvatore; Ferrara, Manuela; Neitzert, Heinrich C.; Rubino, Alfredo; Della Sala, Dario; Vacca, Paolo

CS Dipartimento di Ingegneria Chimica ed Alimentare, Universita di Salerno, Fisciano (Salerno), I-84084, Italy

SO Synthetic Metals (2006), 156(1), 13-20
CODEN: SYMEDZ; ISSN: 0379-6779

PB Elsevier B.V.

DT Journal

LA English

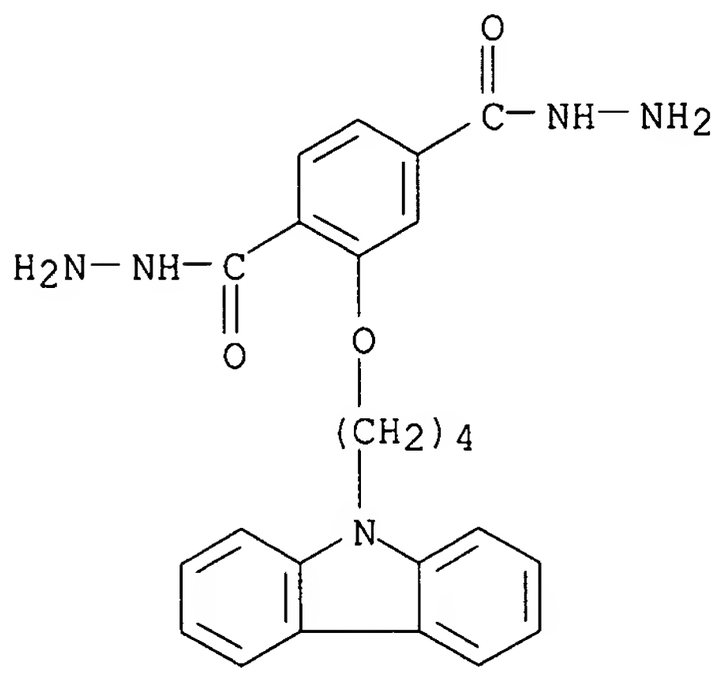
OS CASREACT 144:378247

AB The synthesis of new mols. containing both electron and hole transporter units is reported. This class of compds., named OC, may be used for assembling electroluminescent devices made by a single organic layer. The active moieties are the carbazole, as the hole transporter unit, and the oxadiazole, as the electron transporter unit. The chemical formulation and the complex geometry of the mol. frame allow good solubility in chlorinated solvents and the preparation of homogeneous films by spinning technique. Photoluminescence of mols., both in solution and in film, occurs in the blue region of visible spectra, the exact peak position of emission depending on the pendants attached to the oxadiazole unit. The electroluminescence occurs in a higher wavelength region, with a blue-green emission. The electroluminescent devices consist in the simple sequence ITO-OC-Al and ITO-PEDOT-OC-Al.

IT 881896-43-1P 881896-44-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(benzoylation; synthesis of electroluminescent mols. containing carbazole hole transport and oxadiazole electron transport units for a single-layer blue-emitting OLED)

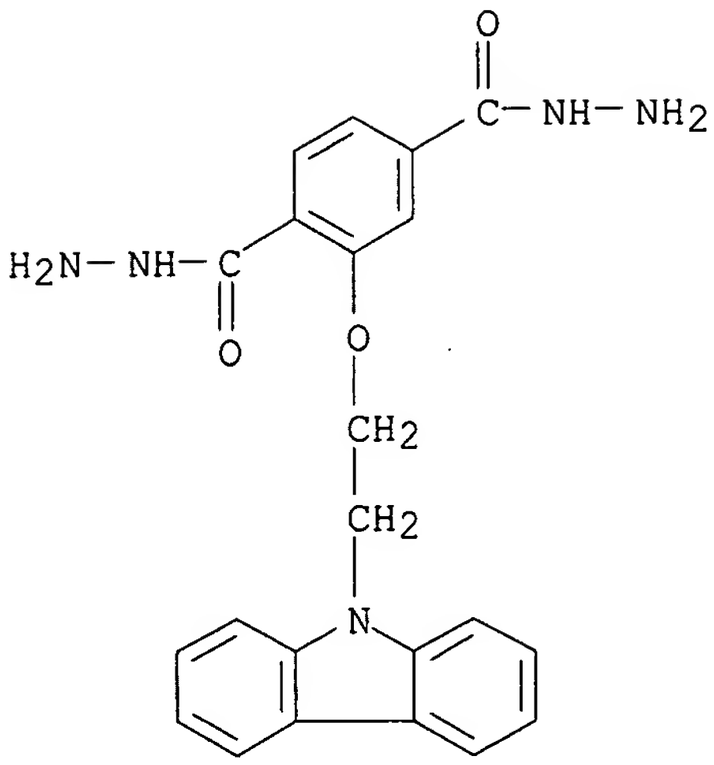
RN 881896-43-1 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-[4-(9H-carbazol-9-yl)butoxy]-, dihydrazide (9CI) (CA INDEX NAME)



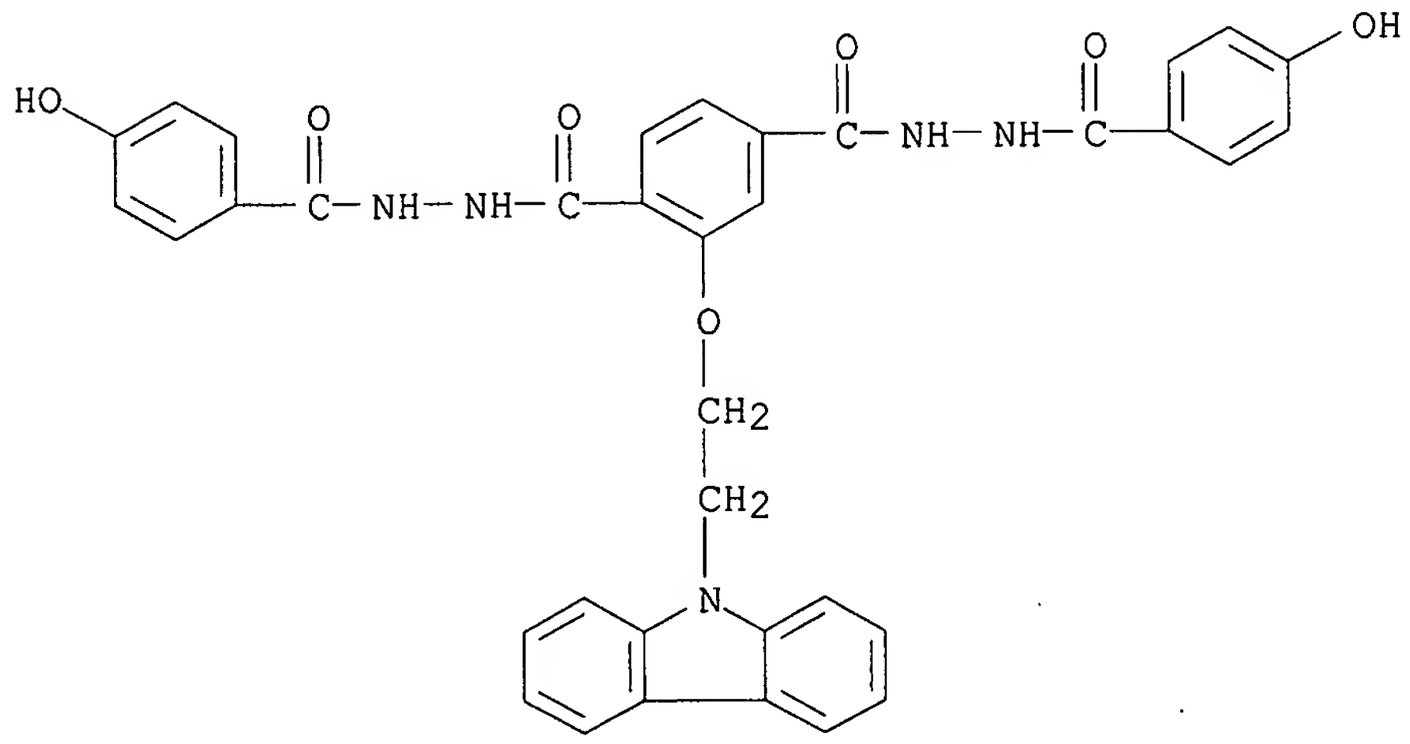
RN 881896-44-2 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-[2-(9H-carbazol-9-yl)ethoxy]-, dihydrazide (9CI) (CA INDEX NAME)

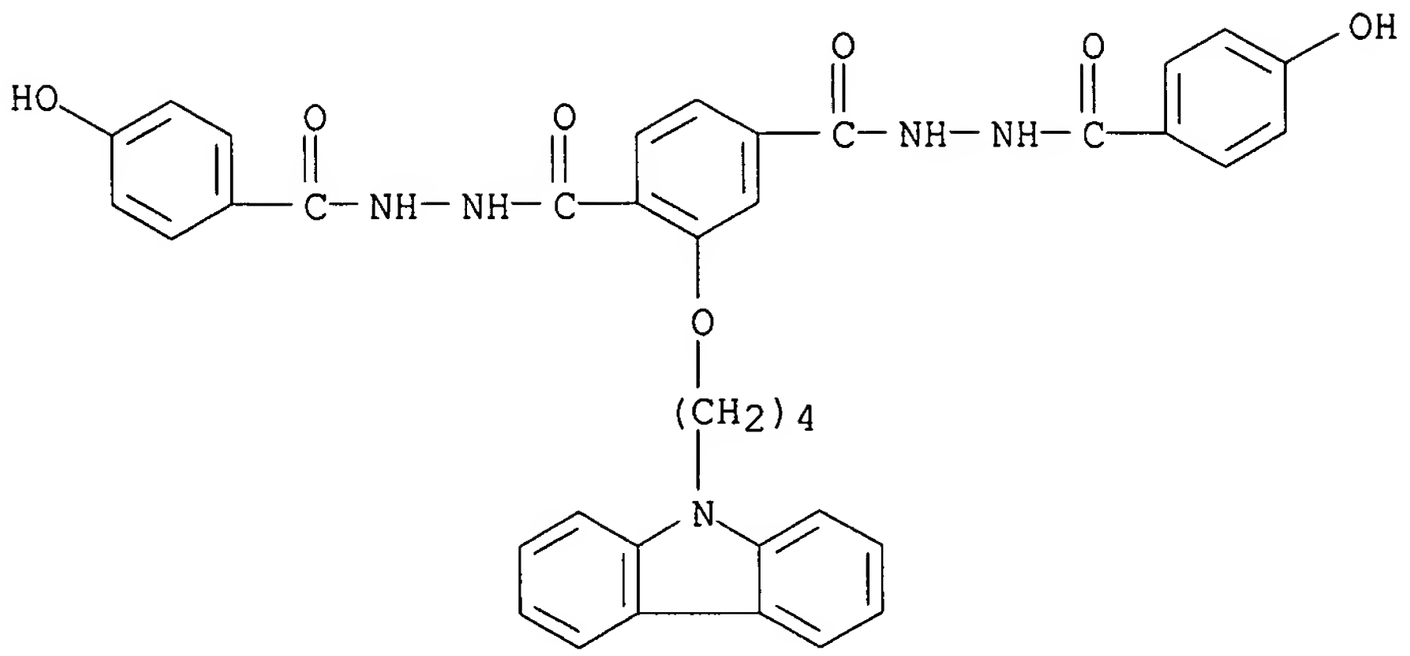


IT 881896-45-3P 881896-46-4P 881896-47-5P
881896-48-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intramol. cyclization and thermal data; synthesis of electroluminescent mols. containing carbazole hole transport and oxadiazole electron transport units for a single-layer blue-emitting OLED)

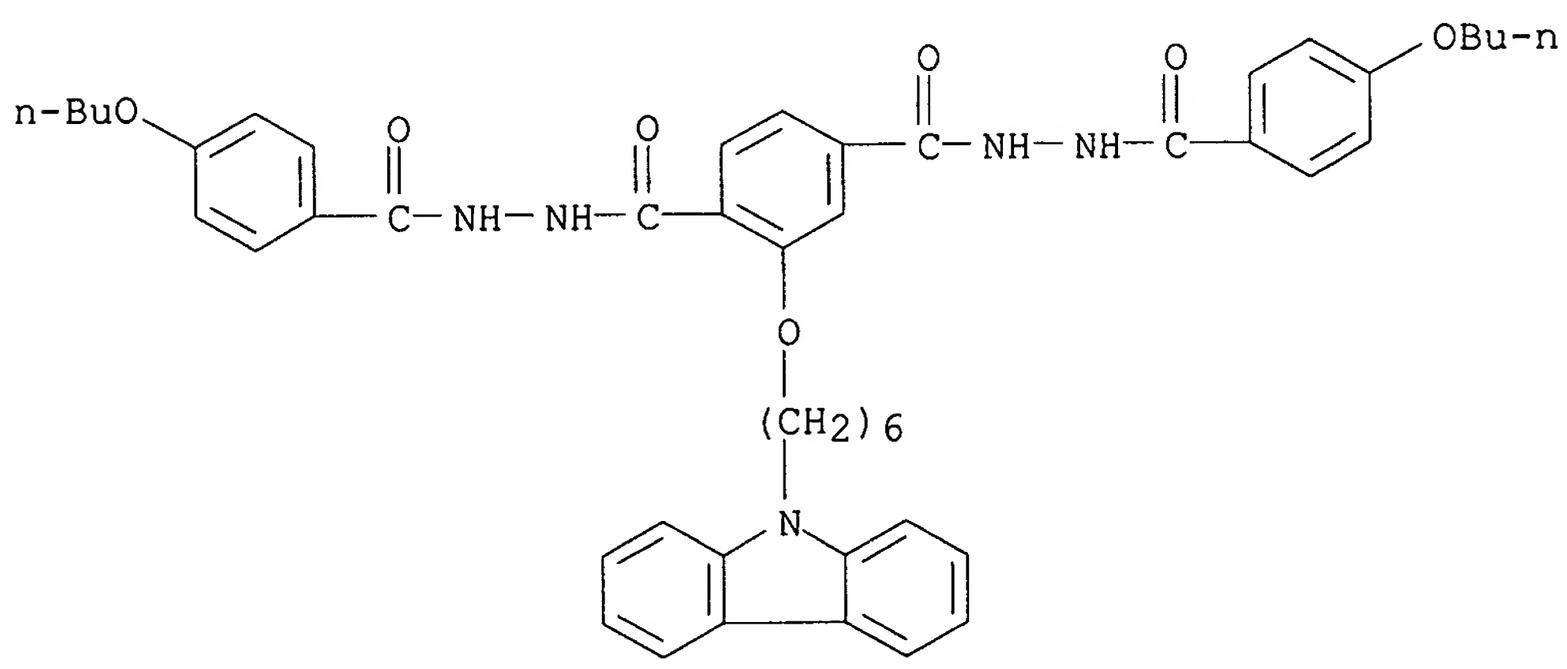
RN 881896-45-3 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-[2-(9H-carbazol-9-yl)ethoxy]-, bis[2-(4-hydroxybenzoyl)hydrazide] (9CI) (CA INDEX NAME)



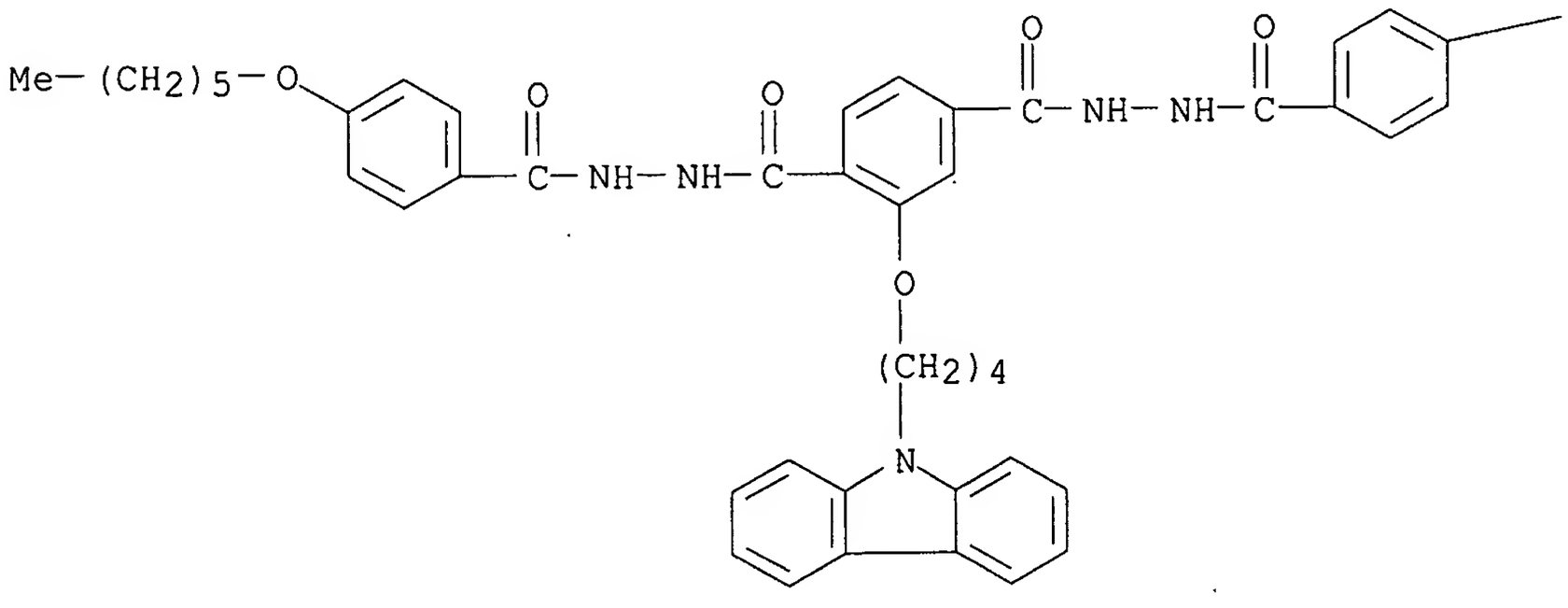
RN 881896-46-4 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-[4-(9H-carbazol-9-yl)butoxy]-, bis[2-(4-hydroxybenzoyl)hydrazide] (9CI) (CA INDEX NAME)



RN 881896-47-5 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-[[6-(9H-carbazol-9-yl)hexyl]oxy]-, bis[2-(4-butoxybenzoyl)hydrazide] (9CI) (CA INDEX NAME)

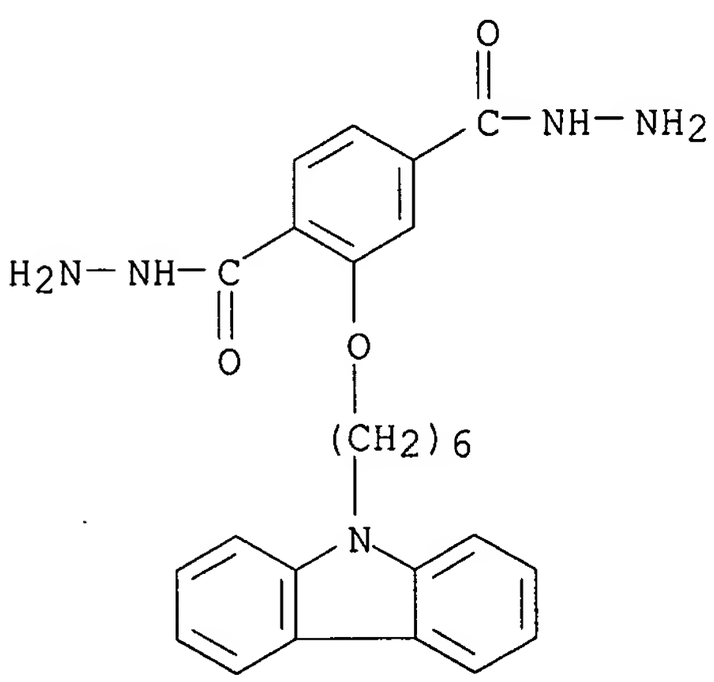


RN 881896-48-6 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-[4-(9H-carbazol-9-yl)butoxy]-, bis[2-[4-(hexyloxy)benzoyl]hydrazide] (9CI) (CA INDEX NAME)



—O—$(CH_2)_5$—Me

IT 924881-57-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of electroluminescent mols. containing carbazole hole transport and oxadiazole electron transport units for a single-layer blue-emitting OLED)
RN 924881-57-2 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-[[6-(9H-carbazol-9-yl)hexyl]oxy]-, 1,4-dihydrazide (CA INDEX NAME)



RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:32921 CAPLUS
DN 144:88556
TI Preparation of tetramines for activation of binding of p53 to DNA
IN Sato, Masakazu; Wada, Hisaya; Amada, Hideaki
PA Taisho Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 36 pp.
CODEN: JKXXAF
DT Patent
LA Japanese

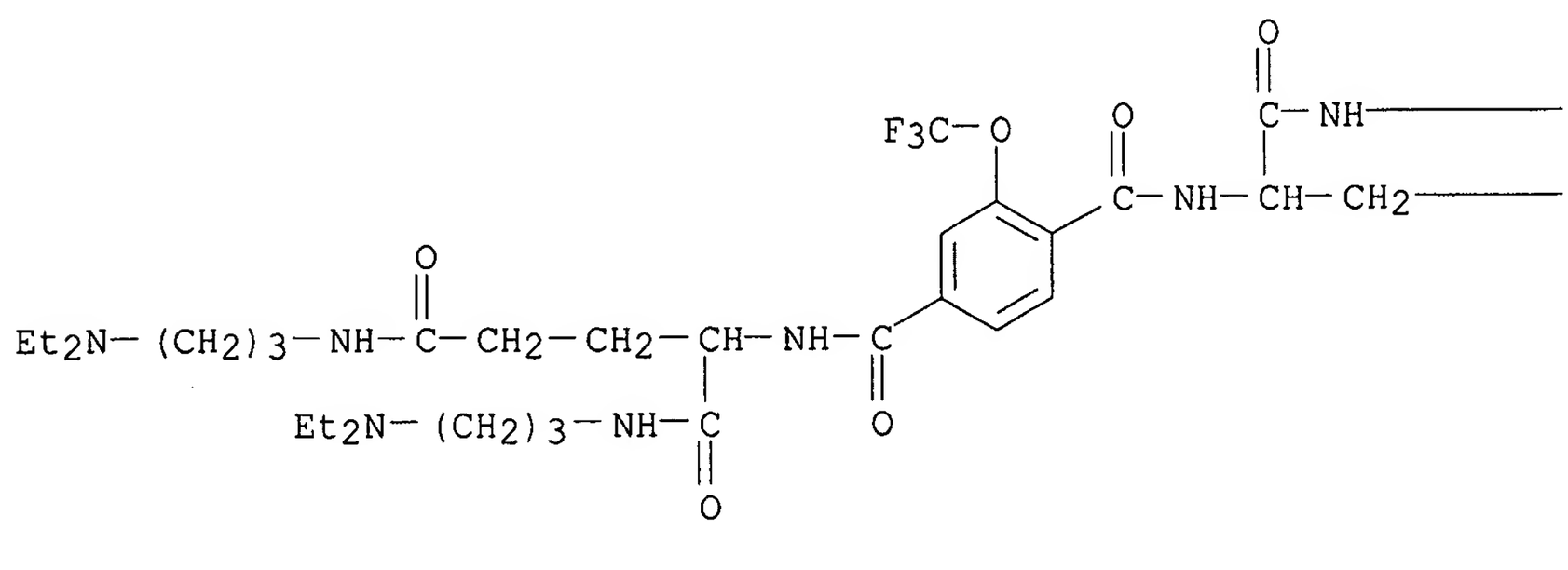
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2006008533	A	20060112	JP 2004-184095	20040622
PRAI JP 2004-184095		20040622		

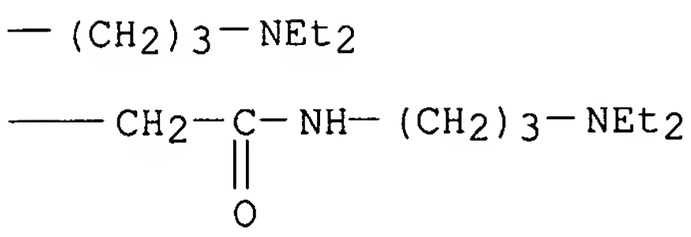
OS MARPAT 144:88556
AB A[CONHCHZ(CH2)mZ]2 [Z = CONH(CH2)nNR1R2; R1, R2 = H, C1-6 alkyl; R1NR2 may form saturated heterocyclyl; n = 1-5; m = 1, 2; A = substituted (cyclo)alkylene, naphthalenediyl, substituted xanthenediyl, etc.] or their medically acceptable salts, useful for induction of apoptosis in tumor cells, are prepared Thus, Z-Glu was amidated with Et2N(CH2)3NH2, deprotected, and refluxed with 2,4,5,6-tetrafluoroisophthaloyl dichloride to give tetramine, which at 100 μM showed 78.4% activation of binding of recombinant human p53 protein to DNA by Pab421 epitope peptide assay.
IT 872461-47-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tetramines as antitumor agents)

RN 872461-47-7 CAPLUS
CN 1,4-Benzenedicarboxamide, N,N'-bis[4-[[3-(diethylamino)propyl]amino]-1-[[[3-(diethylamino)propyl]amino]carbonyl]-4-oxobutyl]-2-(trifluoromethoxy)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L3 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:1334801 CAPLUS
DN 144:69830
TI Preparation of 5-membered heterocycles as serine protease inhibitors for treatment of thromboembolic disorders.
IN Hangeland, Jon J.; Quan, Mimi L.; Smallheer, Joanne M.; Bisacchi, Gregory S.; Corte, James R.; Friends, Todd J.; Sun, Zhong; Rossi, Karen A.; Cavallaro, Cullen L.
PA USA
SO U.S. Pat. Appl. Publ., 166 pp., which
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2005282805	A1	20051222	US 2005-151667	20050613
AU 2005254102	A1	20051229	AU 2005-254102	20050614
CA 2570472	A1	20051229	CA 2005-2570472	20050614
WO 2005123050	A2	20051229	WO 2005-US21212	20050614
WO 2005123050	A3	20070104		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,

EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1773786 A2 20070418 EP 2005-773261 20050614

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU

CN 101006063 A 20070725 CN 2005-80027843 20050614

IN 2006DN07354 A 20070803 IN 2006-DN7354 20061206

KR 2007024601 A 20070302 KR 2006-726365 20061214

NO 2006005864 A 20070302 NO 2006-5864 20061215

PRAI US 2004-579638P P 20040615

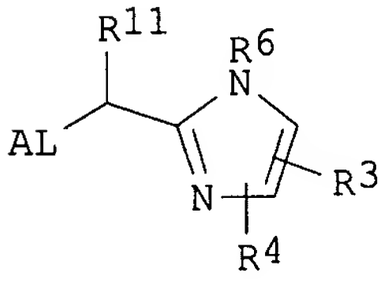
US 2005-684127P P 20050524

US 2005-151667 A 20050613

WO 2005-US21212 W 20050614

OS MARPAT 144:69830

GI



I

AB Title compds. e.g. [I; A = (substituted) carbocyclyl, heterocyclyl; L = CONR10, CH2CONR10, SO2NR10, CH2CH2, CH2O, COCH2, etc.; R3 = (CH2)rCONR8R9, (substituted) carbocyclyl(alkyl), heterocyclyl(alkyl), etc.; R4 = H, F, Cl, Br, iodo, OCF3, cyano, NO2, (substituted) alkyl, alkenyl, alkynyl, carbocyclyl, heterocyclyl, etc.; R6 = H; R8 = H, (substituted) alkyl, phenyl(alkyl), heterocyclylalkyl; R9 = H, (substituted) alkyl, phenyl(alkyl); R10 = H, (substituted) alkyl, alkenyl, alkynyl, carbocyclyl, heterocyclyl; r = 0-4], were prepared Thus, (S)-2-phenyl-1-(4-phenyl-1H-imidazol-2-yl)ethanamine bistrifluoroacetate (preparation given), 4-amidinobenzoic acid hydrochloride, and BOP reagent were stirred in pyridine for 16 h to give 3% (S)-4-carbamimidoyl-N-[2-phenyl-1-(4-phenyl-1H-imidazol-2-yl)ethyl]benzamide. I are useful as selective inhibitors of serine protease enzymes of the coagulation cascade and/or contact activation system such as thrombin, factor Xa, factor XIa, factor IXa, factor VIIa and/or plasma kallikrein; preferred I inhibited these with Ki values of ≤15 μM.

IT 872014-39-6P

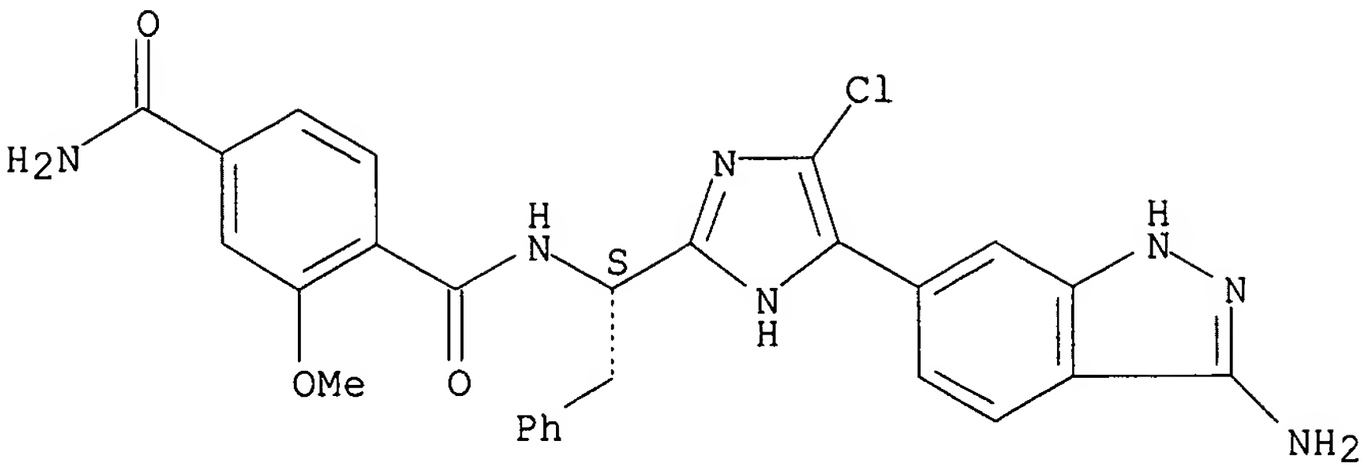
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of 5-membered heterocycles as serine protease inhibitors for treatment of thromboembolic disorders)

RN 872014-39-6 CAPLUS

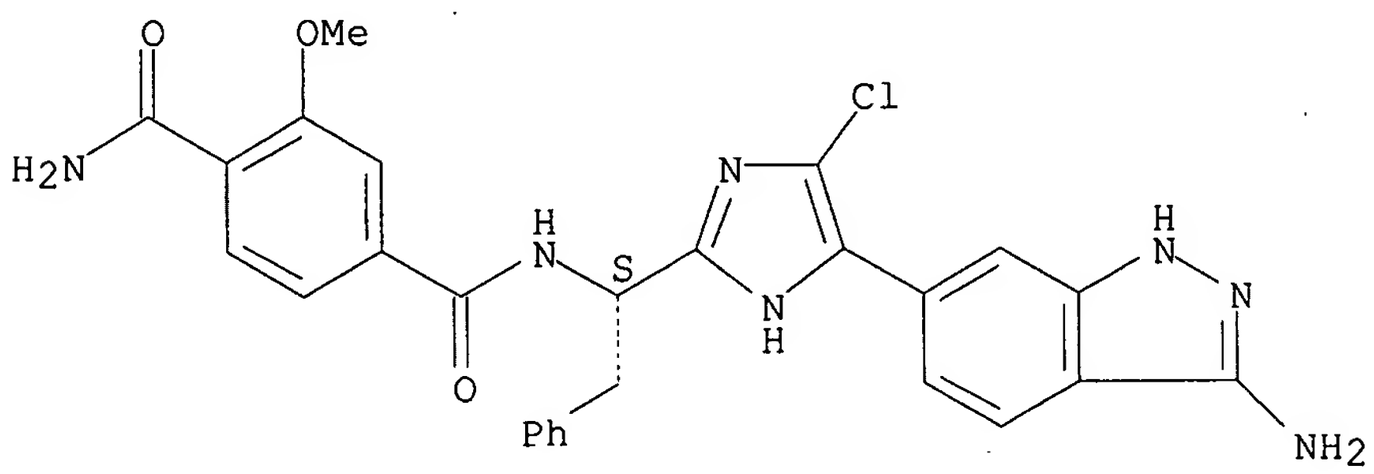
CN 1,4-Benzenedicarboxamide, N1-[(1S)-1-[4-(3-amino-1H-indazol-6-yl)-5-chloro-1H-imidazol-2-yl]-2-phenylethyl]-2-methoxy- (CA INDEX NAME)

Absolute stereochemistry.



IT 872016-44-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 5-membered heterocycles as serine protease inhibitors for treatment of thromboembolic disorders)
RN 872016-44-9 CAPLUS
CN 1,4-Benzenedicarboxamide, N4-[(1S)-1-[4-(3-amino-1H-indazol-6-yl)-5-chloro-1H-imidazol-2-yl]-2-phenylethyl]-2-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

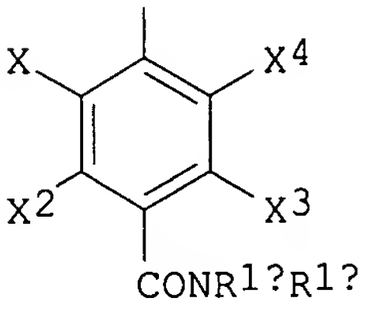


L3 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:961964 CAPLUS
DN 143:248664
TI Preparation of terephthalamide peptidomimetic compounds for therapeutic use
IN Hamilton, Andrew D.; Yin, Hang
PA Yale University, USA
SO PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

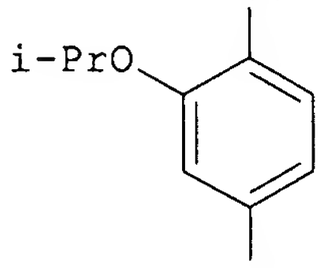
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005079541	A2	20050901	WO 2005-US5557	20050222
	WO 2005079541	A3	20051103		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,

RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG
AU 2005215051 A1 20050901 AU 2005-215051 20050222
CA 2556447 A1 20050901 CA 2005-2556447 20050222
EP 1723100 A2 20061122 EP 2005-713917 20050222
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA,
HR, LV, MK, YU
US 2007123592 A1 20070531 US 2006-588478 20061002
PRAI US 2004-546111P P 20040219
WO 2005-US5557 W 20050222
OS CASREACT 143:248664; MARPAT 143:248664
GI



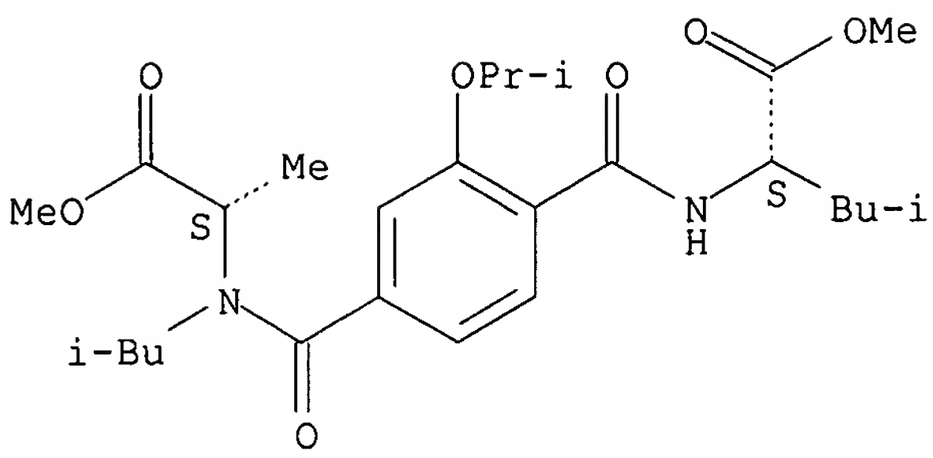
I



II

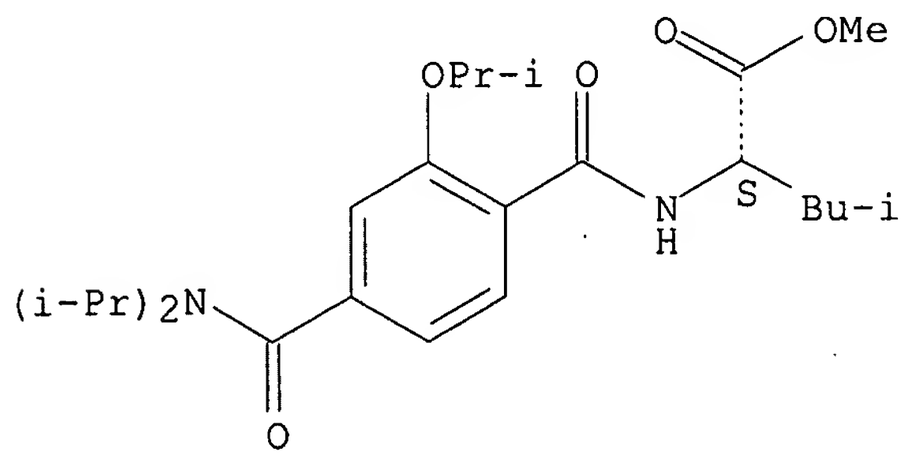
AB The invention relates to compds. and pharmaceutical compns. based on terephthalamide which are proteomimetic and methods for inhibiting the interaction of an α-helical protein with another protein or binding site and for treating diseases or conditions which are modulated through these interactions. Compds. I [X is H, halo, R, OR, SR or an amino group, where R is H, (un)substituted alkyl, acyl, aryl, heteroaryl, alkylenearyl or alkyleneheteroaryl; X2, X3, X4 are independently H, halo, OH, Rc, ORc, where Rc is (un)substituted alkyl, acyl, aryl or alkylenearyl; R4 is H, (un)substituted alkyl, alkenyl or alkylene amine; R', R1a, R1b are any group given for R4 or (CH2)0-2CHR2CO2H or an alkyl ester, where R2 is independently H or (un)substituted hydrocarbon, alkoxy, ester, alkanol, alkanoic acid, amine, etc.; or N-R' or NR1aR1b form an amino acid residue] are claimed. Thus, peptidomimetic compound II, prepared via coupling reaction of L-leucine Me ester hydrochloride, showed inhibitory constant Ki = 0.781 ± 0.070 μM in a fluorescence polarization assay (binding affinity for Bcl-XL).
IT 681466-00-2P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(conformation; preparation of terephthalamide peptidomimetic compds. for therapeutic use)
RN 681466-00-2 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-2-methoxy-1-methyl-2-oxoethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



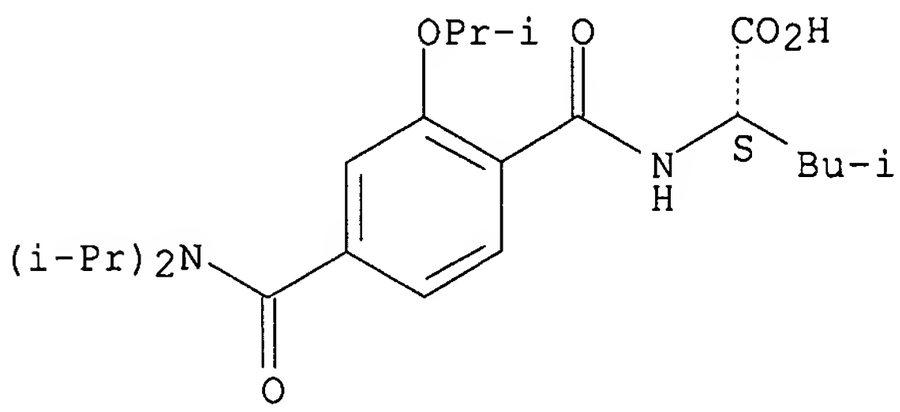
IT 681465-54-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of terephthalamide peptidomimetic compds. for therapeutic use)
RN 681465-54-3 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 681465-56-5P 681465-60-1P 681465-62-3P
681465-68-9P 681465-70-3P 681465-74-7P
852065-21-5P 852065-22-6P 852065-26-0P
852065-27-1P 852065-28-2P 852065-29-3P
852065-30-6P 852065-31-7P 852065-32-8P
852065-33-9P 852065-34-0P 852065-35-1P
852065-36-2P 852065-37-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of terephthalamide peptidomimetic compds. for therapeutic use)
RN 681465-56-5 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

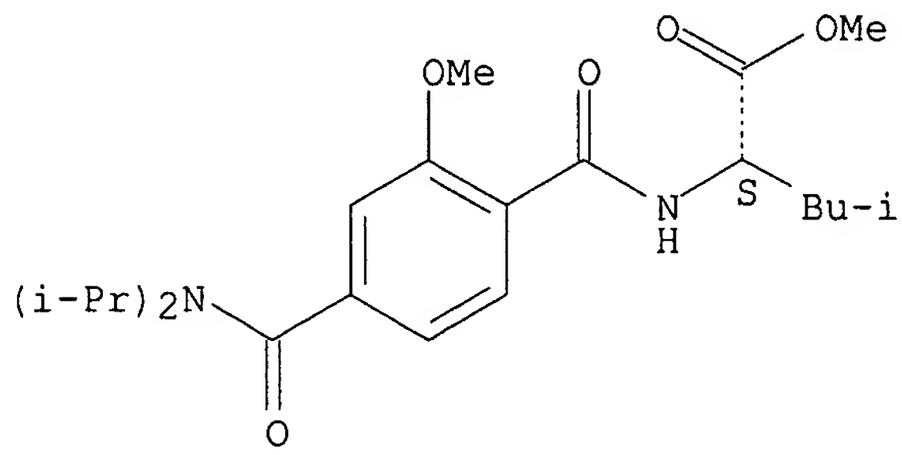
Absolute stereochemistry.



RN 681465-60-1 CAPLUS

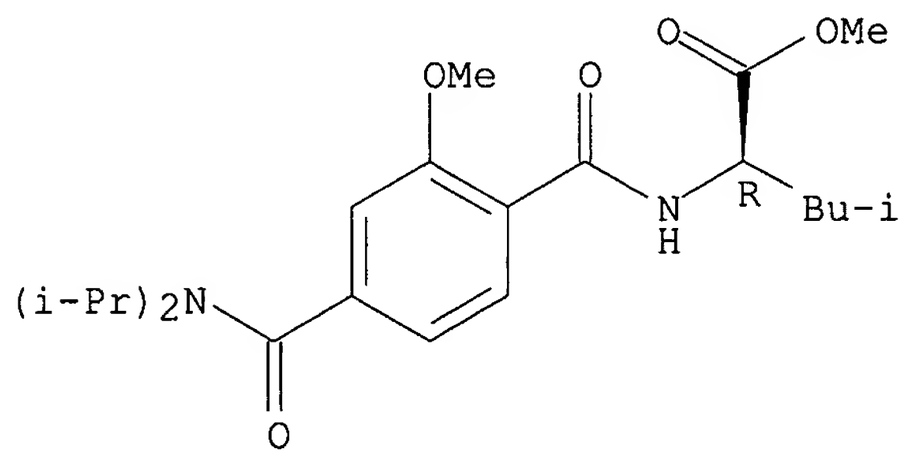
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



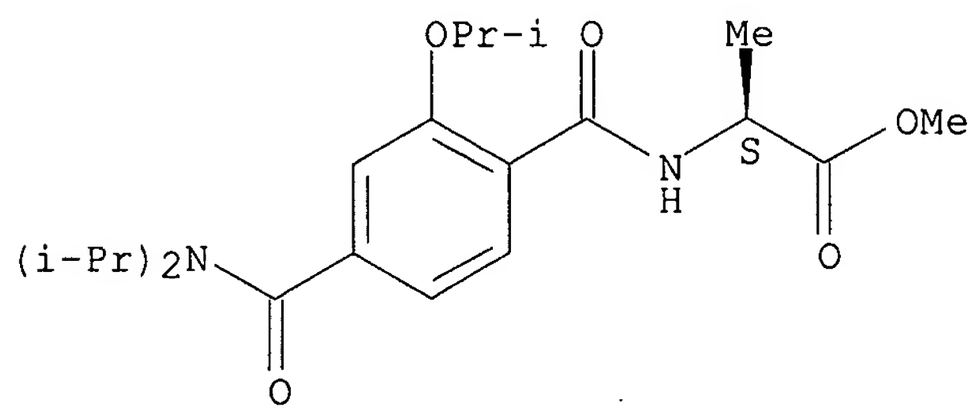
RN 681465-62-3 CAPLUS
CN D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



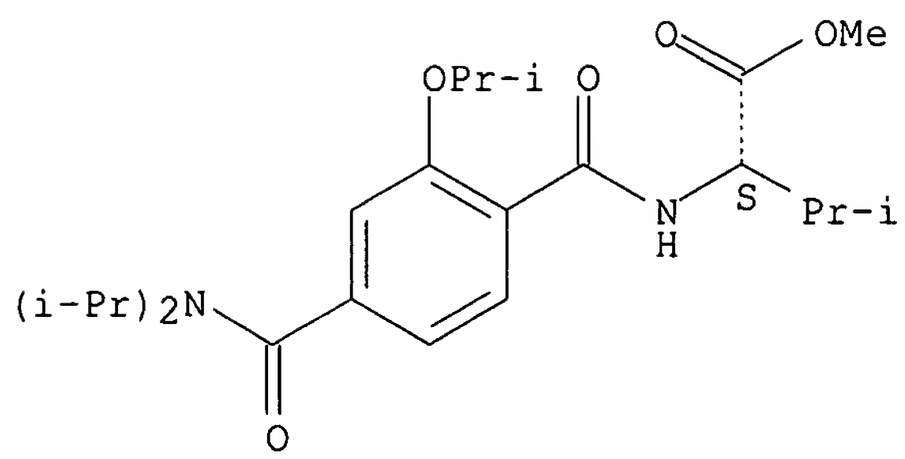
RN 681465-68-9 CAPLUS
CN L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



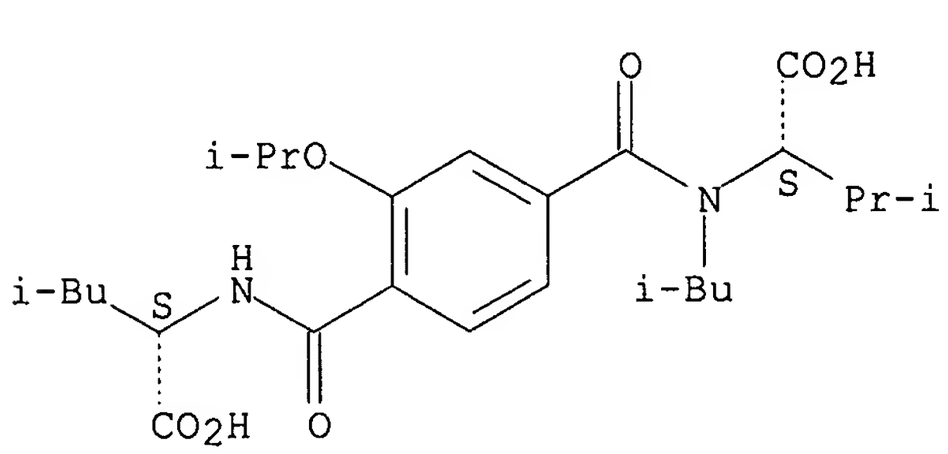
RN 681465-70-3 CAPLUS
CN L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



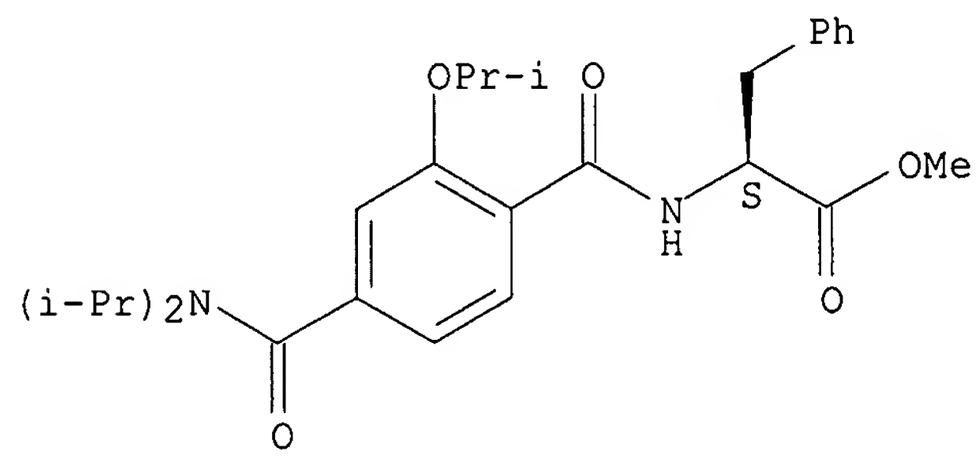
RN 681465-74-7 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



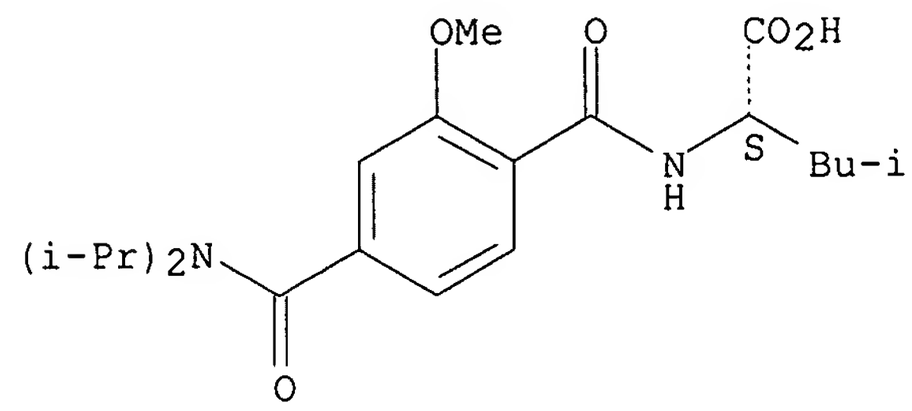
RN 852065-21-5 CAPLUS
CN L-Phenylalanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



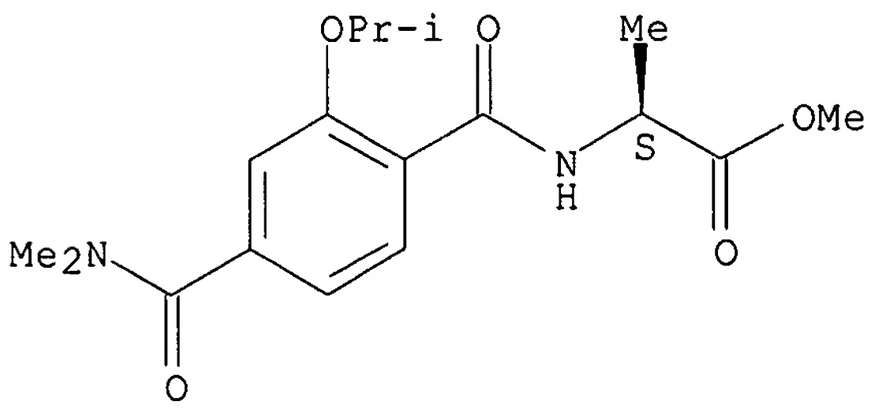
RN 852065-22-6 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



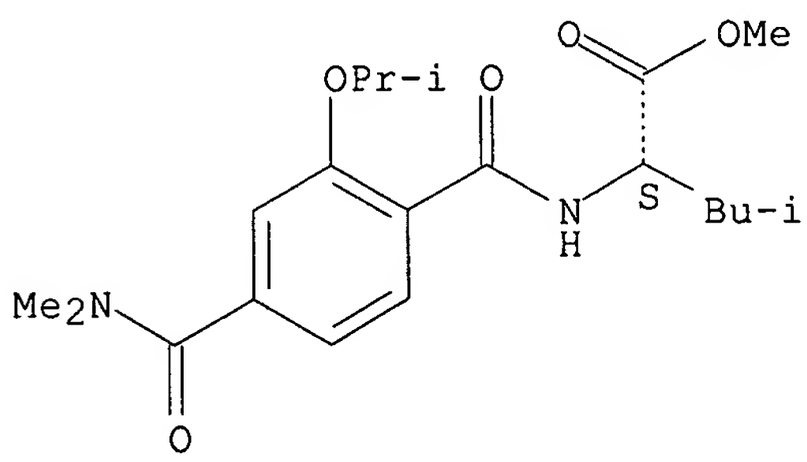
RN 852065-26-0 CAPLUS
CN L-Alanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



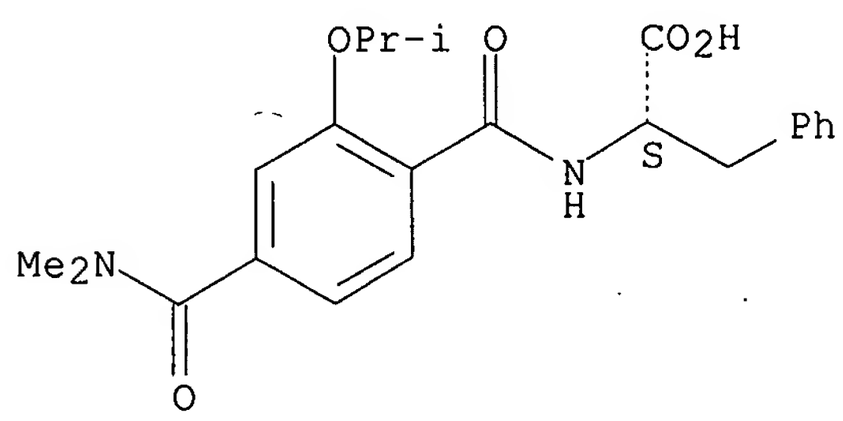
RN 852065-27-1 CAPLUS
CN L-Leucine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



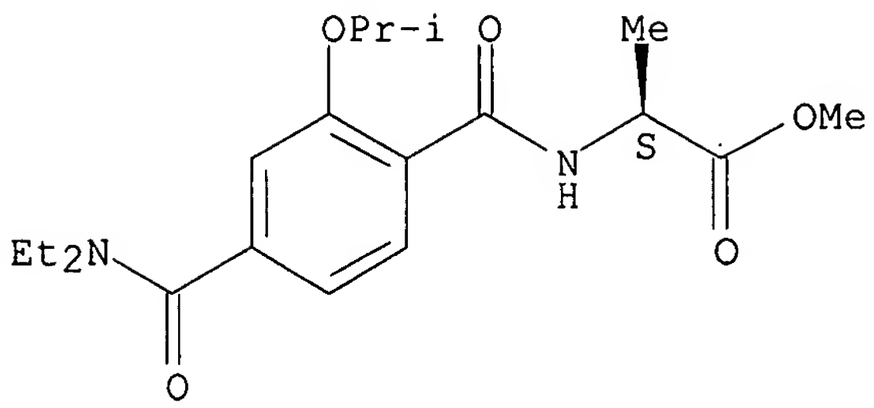
RN 852065-28-2 CAPLUS
CN L-Phenylalanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



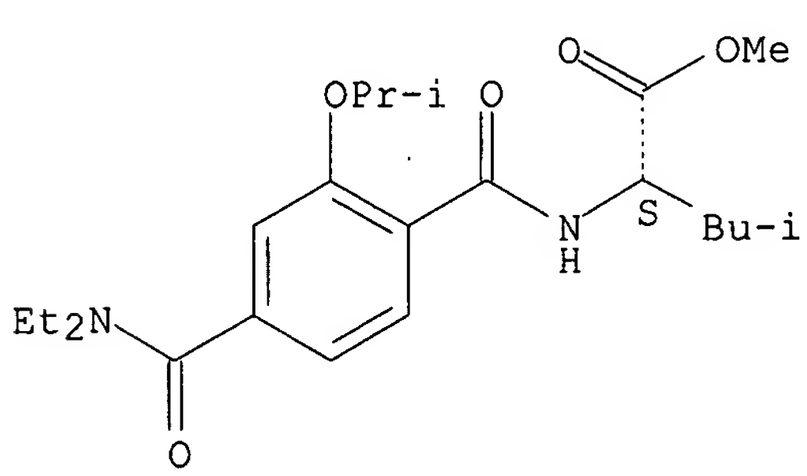
RN 852065-29-3 CAPLUS
CN L-Alanine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



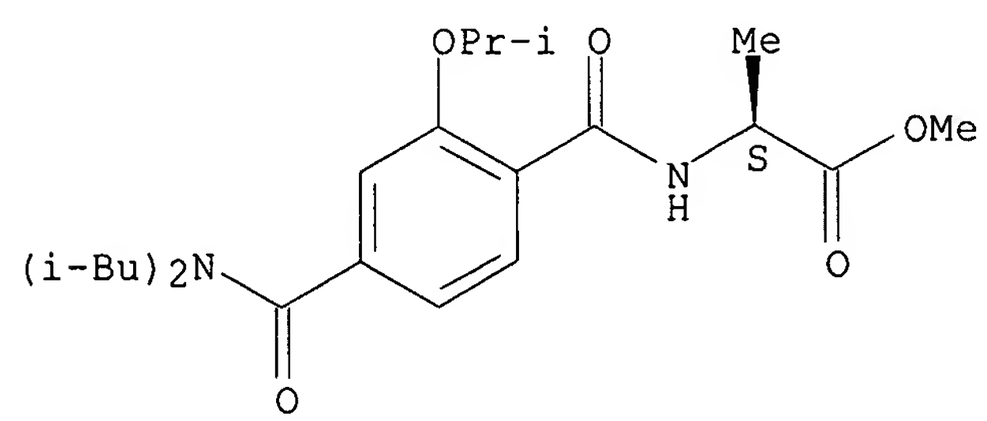
RN 852065-30-6 CAPLUS
CN L-Leucine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



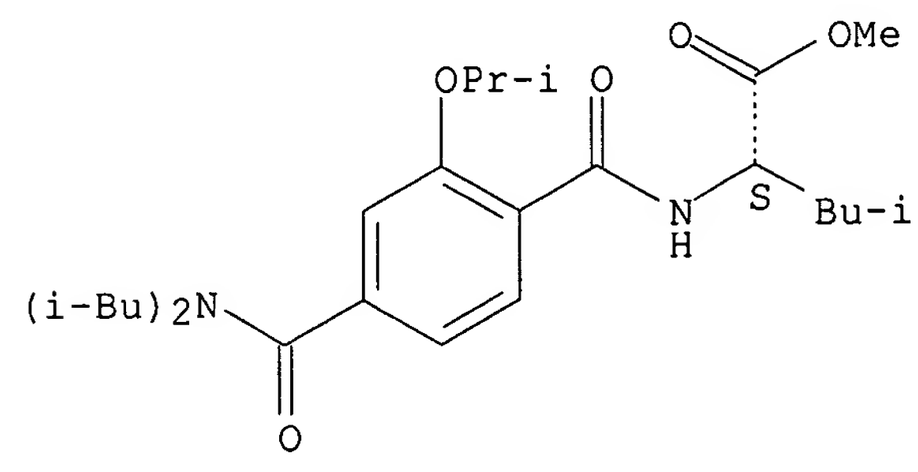
RN 852065-31-7 CAPLUS
CN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



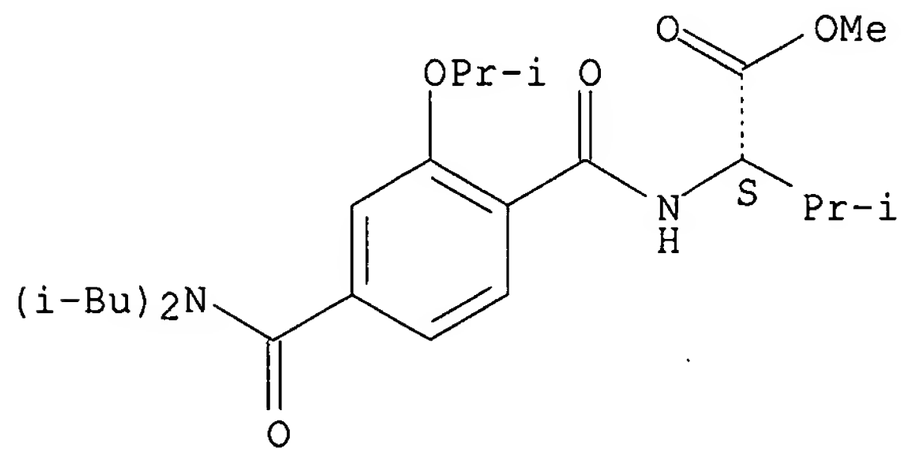
RN 852065-32-8 CAPLUS
CN L-Leucine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



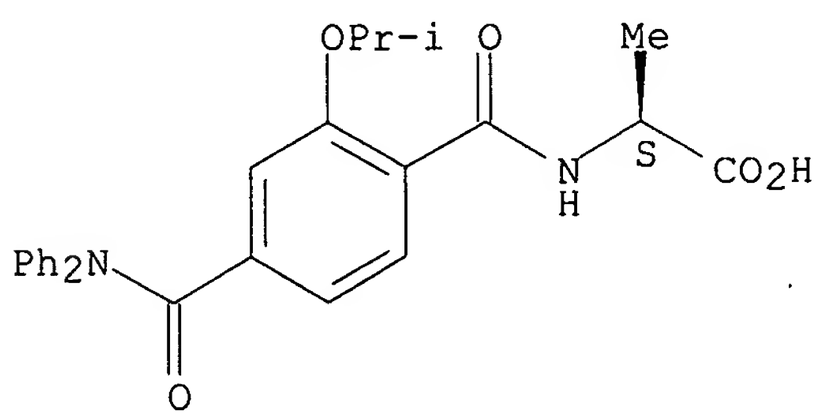
RN 852065-33-9 CAPLUS
CN L-Valine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



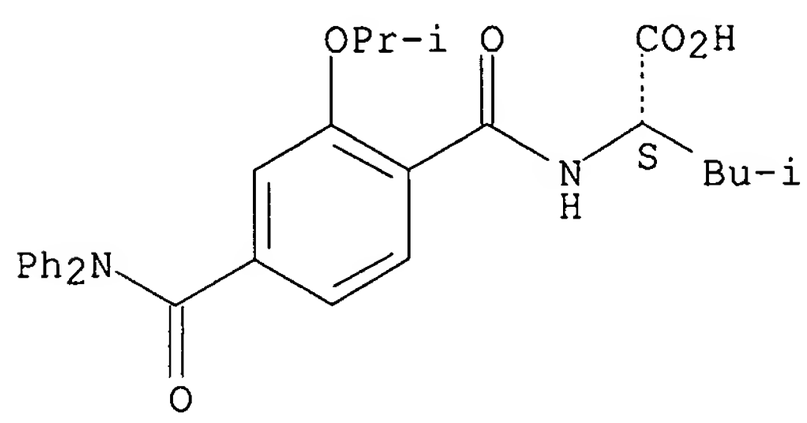
RN 852065-34-0 CAPLUS
CN L-Alanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



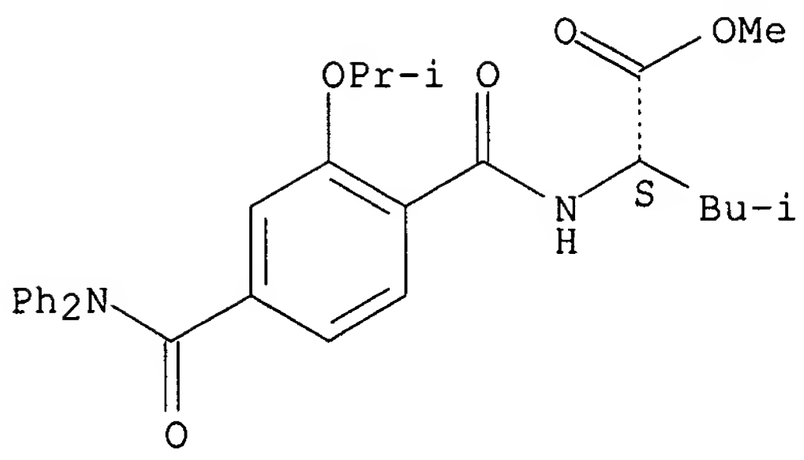
RN 852065-35-1 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



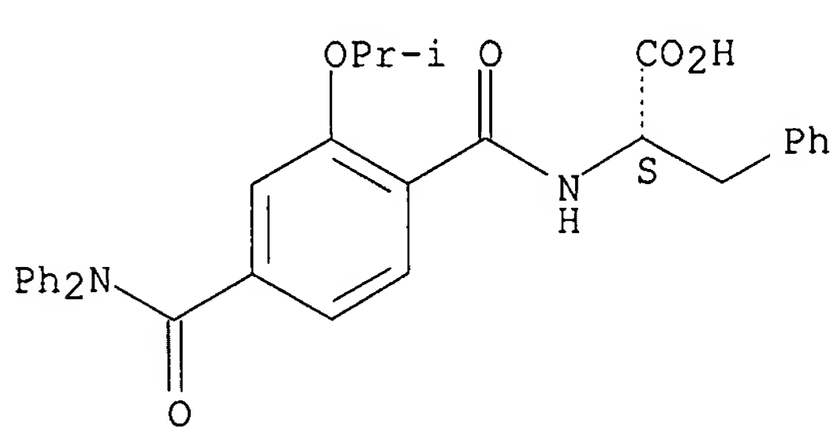
RN 852065-36-2 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 852065-37-3 CAPLUS
CN L-Phenylalanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



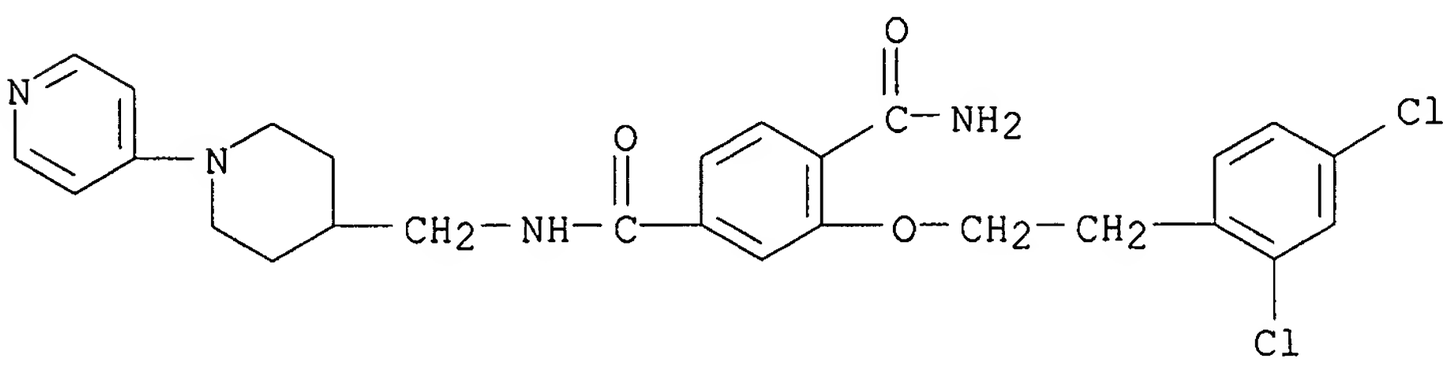
L3 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:312873 CAPLUS
DN 143:39922
TI Structural Requirements for Factor Xa Inhibition by 3-Oxybenzamides with Neutral P1 Substituents: Combining X-ray Crystallography, 3D-QSAR, and Tailored Scoring Functions
AU Matter, Hans; Will, David W.; Nazare, Marc; Schreuder, Herman; Laux, Volker; Wehner, Volkmar
CS DIA Chemistry, Aventis Pharma Deutschland GmbH, Frankfurt am Main, D-65926, Germany
SO Journal of Medicinal Chemistry (2005), 48(9), 3290-3312
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB The design, synthesis, and structure-activity relationship of 3-oxybenzamides as potent inhibitors of the coagulation protease factor Xa are described on the basis of X-ray structures, privileged structure motifs, and SAR information. A total of six x-ray structures of fXa/inhibitor complexes led us to identify the major protein-ligand interactions. The binding mode is characterized by a lipophilic dichlorophenyl substituent interacting with Tyr228 in the protease S1 pocket, while polar parts are accommodated in S4. This alignment in combination with docking allowed derivation of 3D-QSAR models and tailored scoring functions to rationalize biol. affinity and provide guidelines for optimization. The resulting models showed good correlation coeffs. and predictions of external test sets. Furthermore, they correspond to binding site topologies in terms of steric, electrostatic, and hydrophobic complementarity. Two approaches to derive tailored scoring functions combining binding site and ligand information led to predictive models with acceptable predictions of the external set. Good correlations to exptl. affinities were obtained for both AFMoC (adaptation of fields for mol. comparison) and the novel TScore function. The SAR information from 3D-QSAR and tailored scoring functions agrees with all exptl. data and

provides guidelines and reasonable activity estns. for novel fXa inhibitors.

IT 717902-18-6
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(structural requirements for factor Xa inhibition by 3-oxybenzamides with neutral P1 substituents)

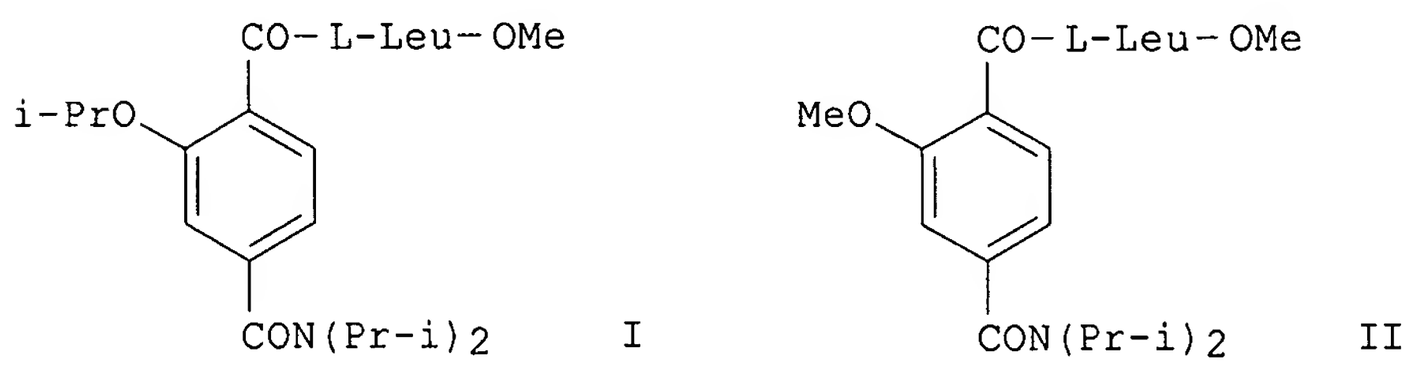
RN 717902-18-6 CAPLUS

CN 1,4-Benzenedicarboxamide, 2-[2-(2,4-dichlorophenyl)ethoxy]-N4-[[1-(4-pyridinyl)-4-piperidinyl]methyl]- (CA INDEX NAME)



RE.CNT 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:267006 CAPLUS
DN 142:482288
TI Terephthalamide Derivatives as Mimetics of Helical Peptides: Disruption of the Bcl-xL/Bak Interaction
AU Yin, Hang; Lee, Gui-in; Sedey, Kristine A.; Rodriguez, Johanna M.; Wang, Hong-Gang; Sebti, Said M.; Hamilton, Andrew D.
CS Department of Chemistry, Yale University, New Haven, CT, 06520-8107, USA
SO Journal of the American Chemical Society (2005), 127(15), 5463-5468
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 142:482288
GI



I

II

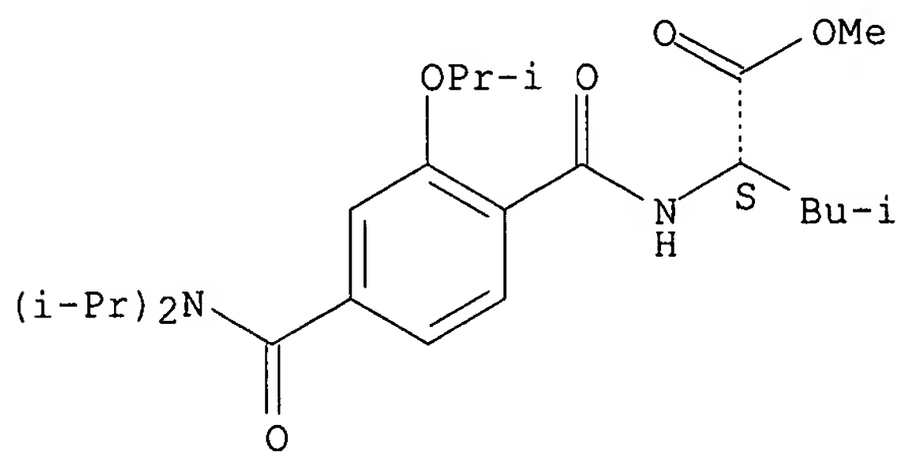
AB A series of Bcl-xL/Bak antagonists, based on a terephthalamide scaffold, was designed to mimic the α-helical region of the Bak peptide. These mols. showed favorable in-vitro activities in disrupting the Bcl-xL/Bak BH3 domain complex (terephthalamides I and II, Ki = 0.78 ± 0.07 and 1.85 ± 0.32 μM, resp.). Extensive structure-affinity studies demonstrated a correlation between the ability of terephthalamide derivs. to disrupt Bcl-xL/Bak complex formation and the size of variable side chains on these mols. Treatment of human HEK293 cells with the terephthalamide derivative 26 resulted in disruption of the Bcl-xL/Bax interaction in whole cells with an IC50 of 35.0 μM. Computational docking simulations and NMR expts. suggested that the binding cleft for

the BH3 domain of the Bak peptide on the surface of Bcl-xL is the target area for these synthetic inhibitors.

IT 681465-54-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of terephthalamide derivs. as helical peptidomimetics and their evaluation as antagonists of Bcl-x/Bak protein interaction)

RN 681465-54-3 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

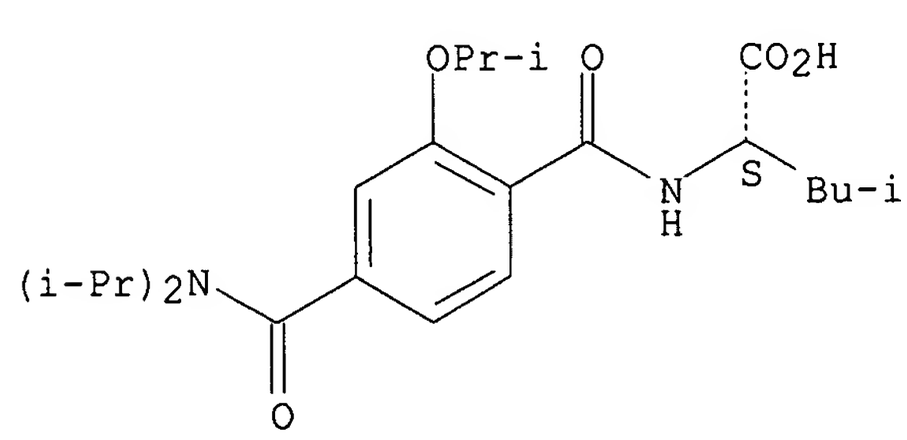
Absolute stereochemistry. Rotation (-).



IT 681465-56-5P 681465-58-7P 681465-60-1P
681465-62-3P 681465-68-9P 681465-70-3P
681465-74-7P 852065-21-5P 852065-22-6P
852065-26-0P 852065-27-1P 852065-28-2P
852065-29-3P 852065-30-6P 852065-31-7P
852065-32-8P 852065-33-9P 852065-34-0P
852065-35-1P 852065-36-2P 852065-37-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of terephthalamide derivs. as helical peptidomimetics and their evaluation as antagonists of Bcl-x/Bak protein interaction)

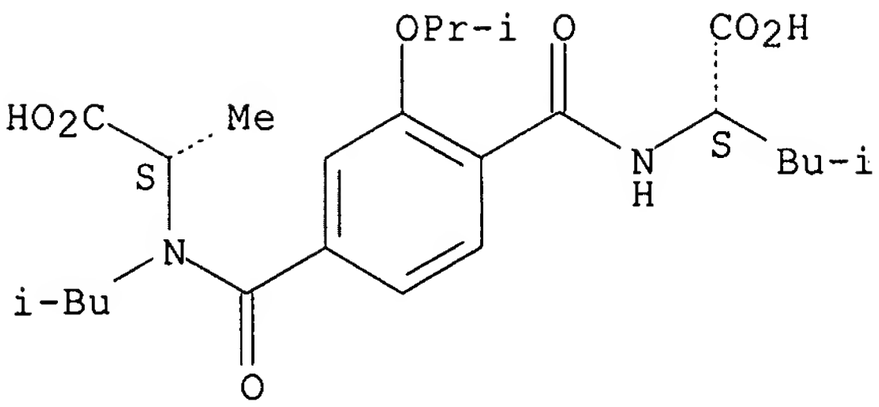
RN 681465-56-5 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



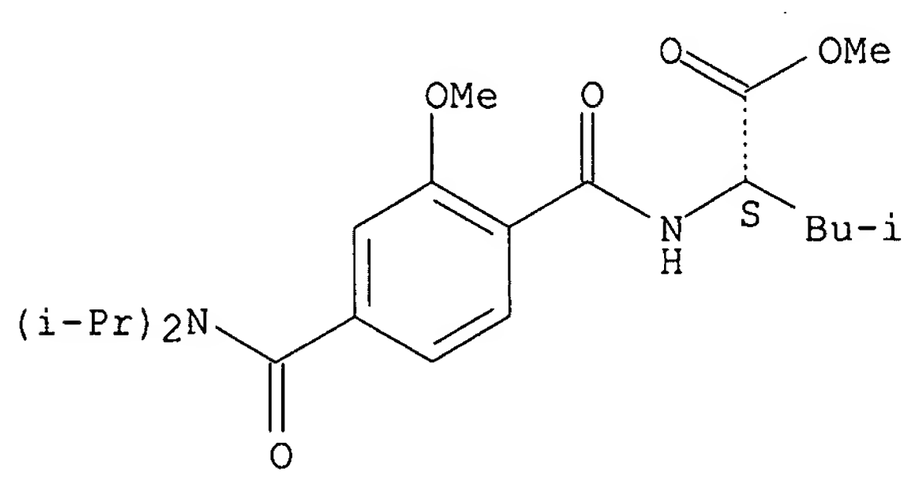
RN 681465-58-7 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-1-carboxyethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



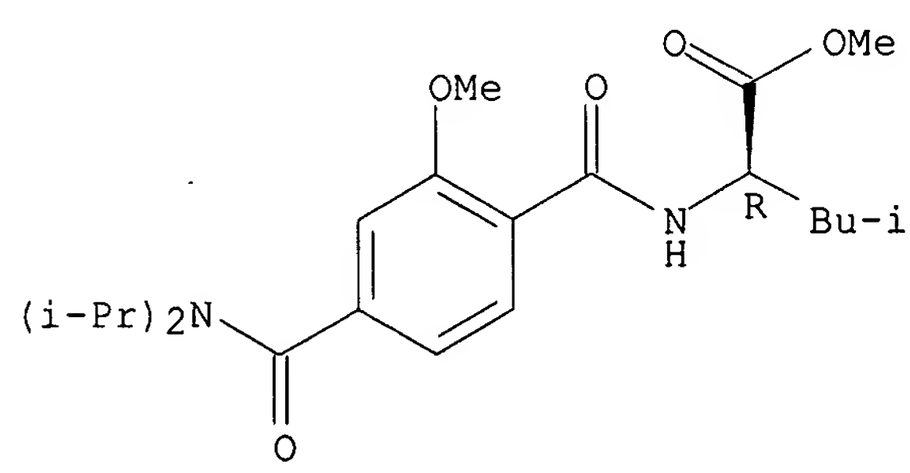
RN 681465-60-1 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



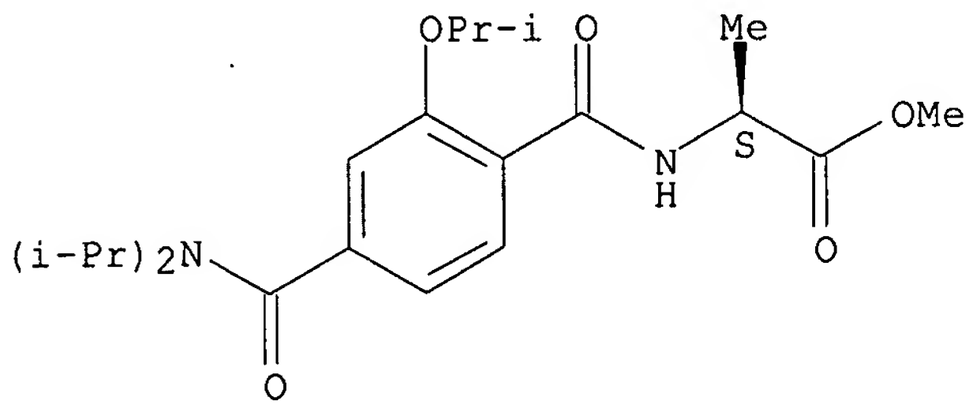
RN 681465-62-3 CAPLUS
CN D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



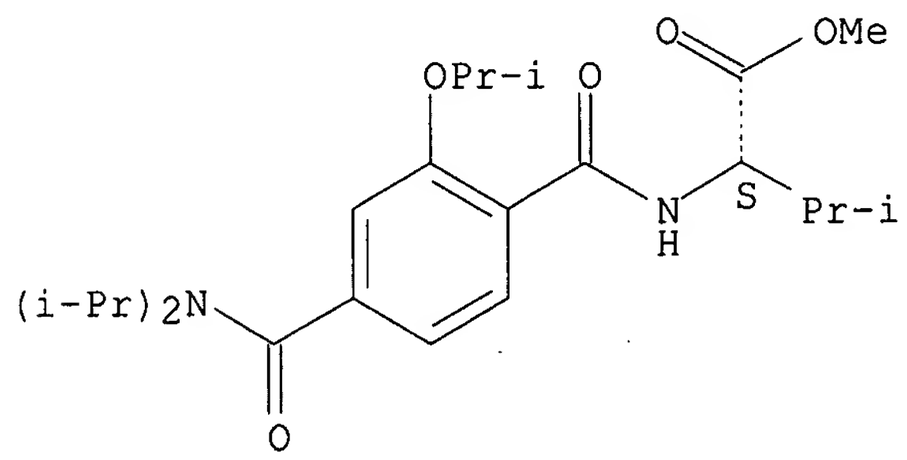
RN 681465-68-9 CAPLUS
CN L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



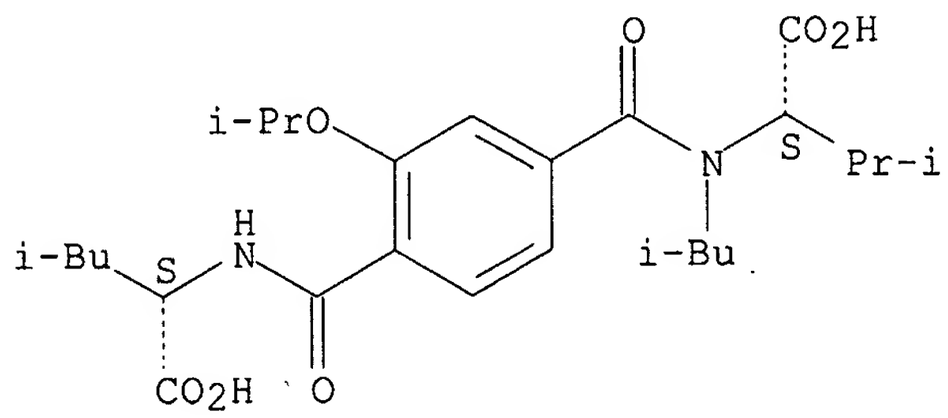
RN 681465-70-3 CAPLUS
CN L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



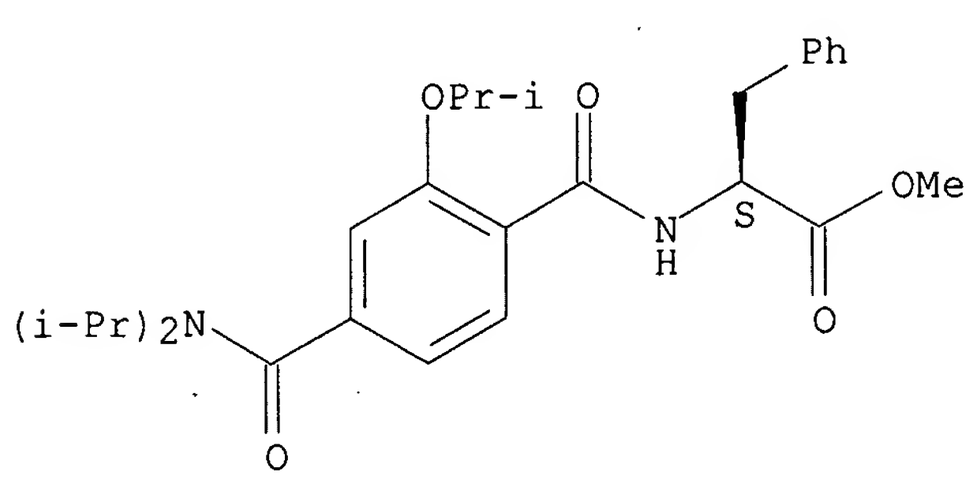
RN 681465-74-7 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



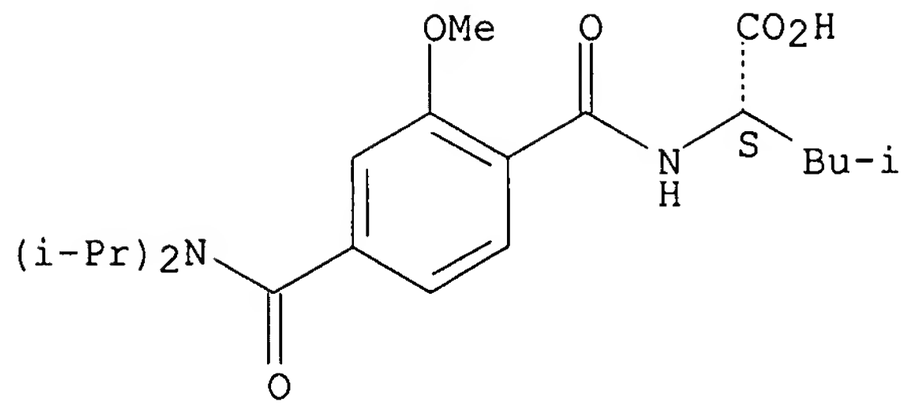
RN 852065-21-5 CAPLUS
CN L-Phenylalanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



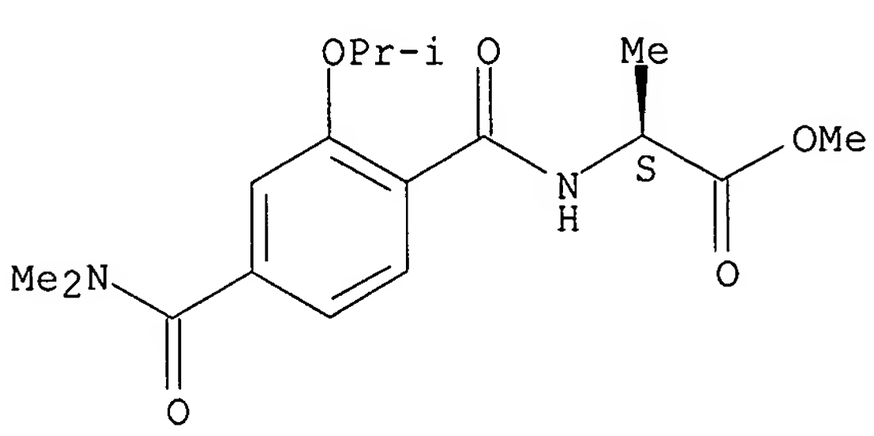
RN 852065-22-6 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



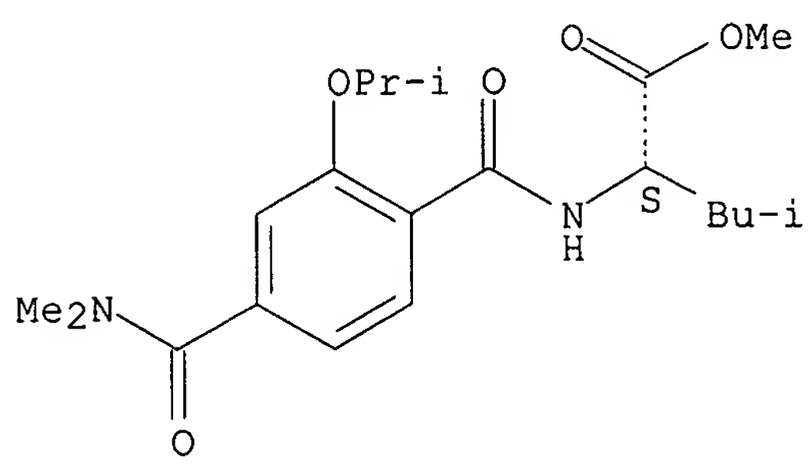
RN 852065-26-0 CAPLUS
CN L-Alanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



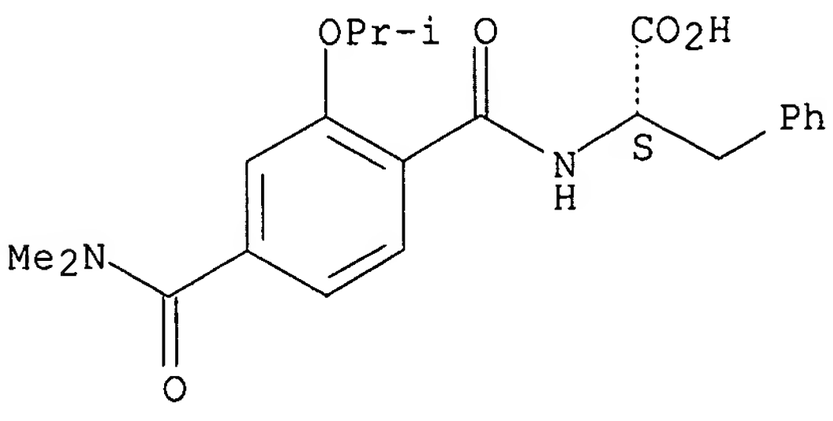
RN 852065-27-1 CAPLUS
CN L-Leucine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 852065-28-2 CAPLUS
CN L-Phenylalanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

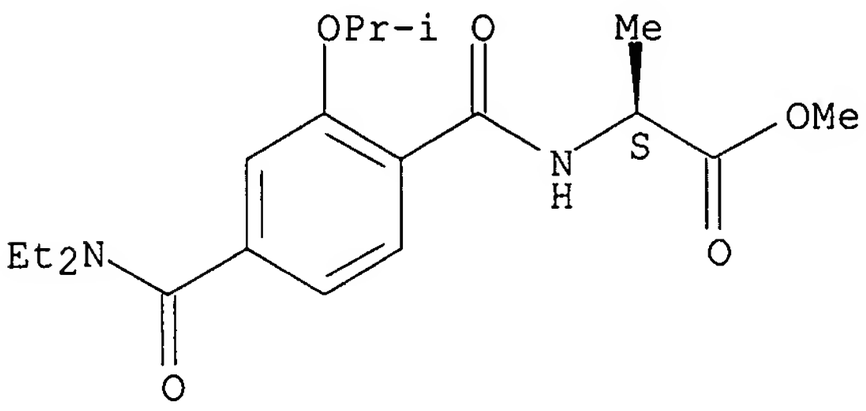
Absolute stereochemistry. Rotation (+).



RN 852065-29-3 CAPLUS

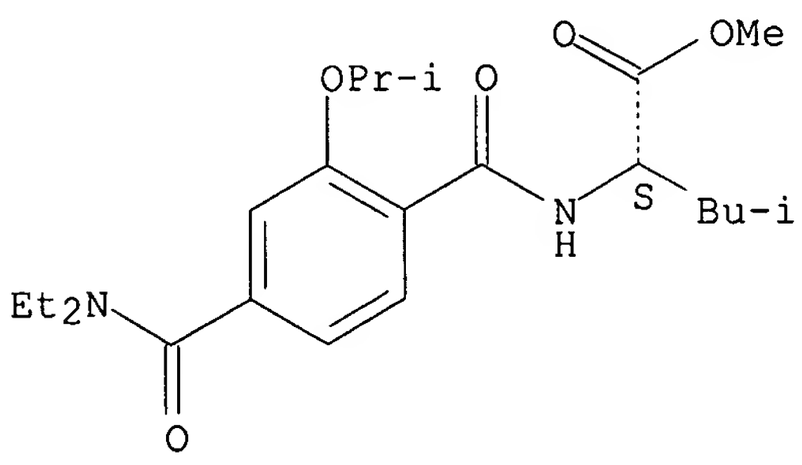
CN L-Alanine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



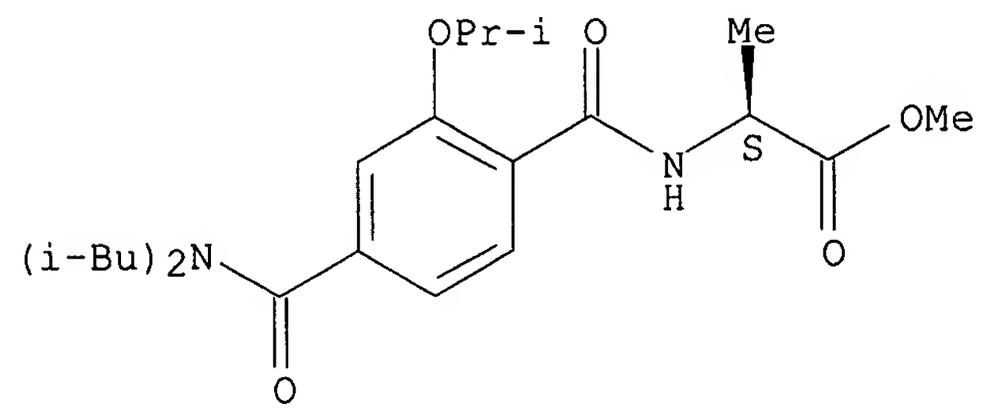
RN 852065-30-6 CAPLUS
CN L-Leucine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



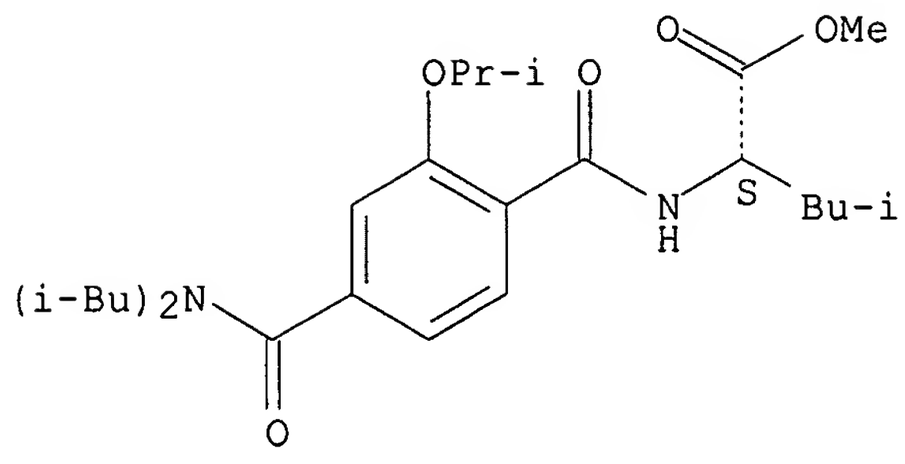
RN 852065-31-7 CAPLUS
CN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



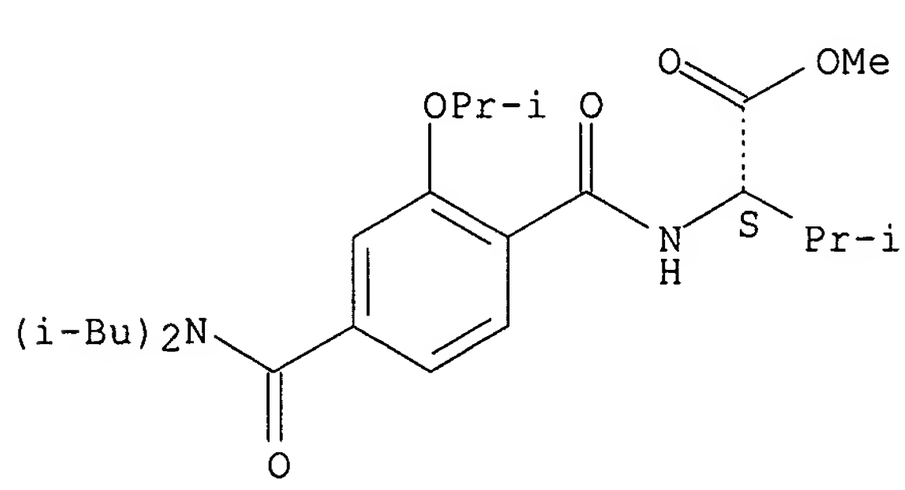
RN 852065-32-8 CAPLUS
CN L-Leucine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



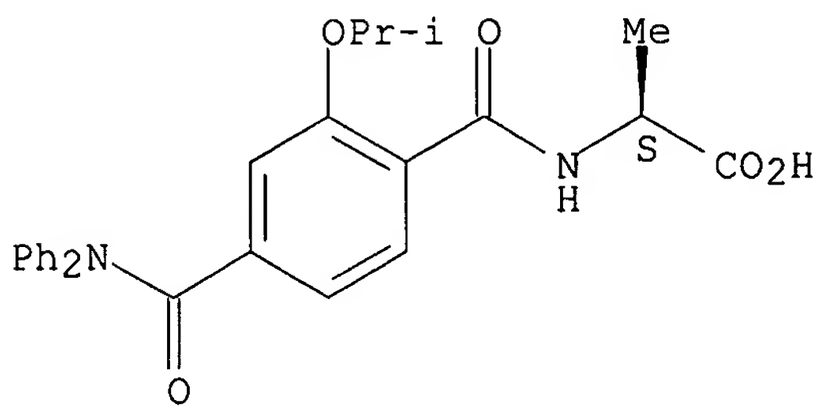
RN 852065-33-9 CAPLUS
CN L-Valine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



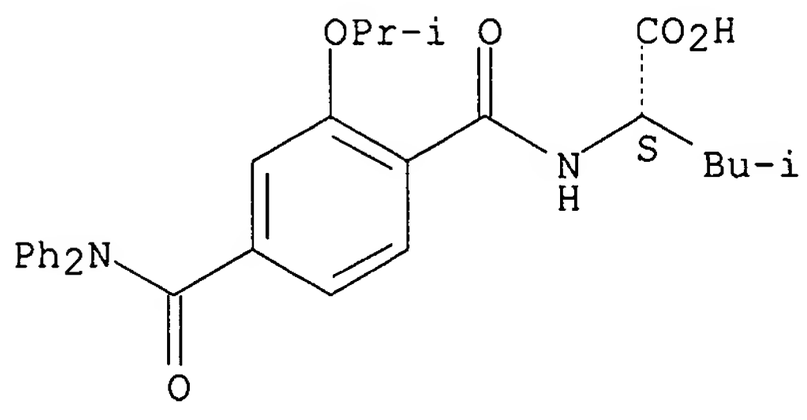
RN 852065-34-0 CAPLUS
CN L-Alanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



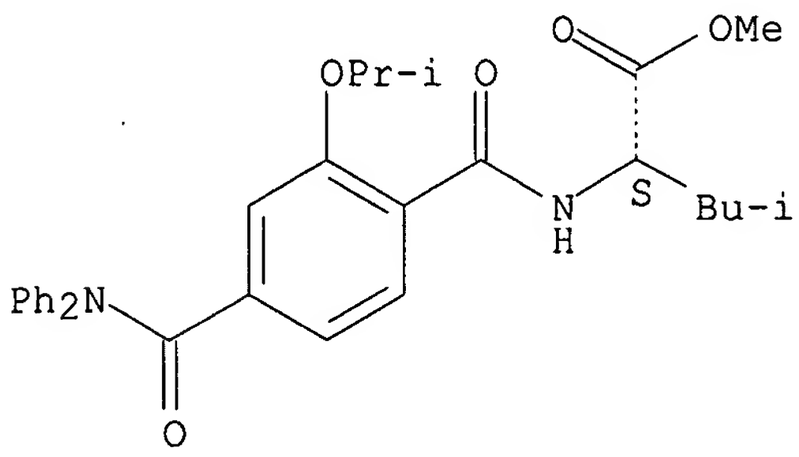
RN 852065-35-1 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



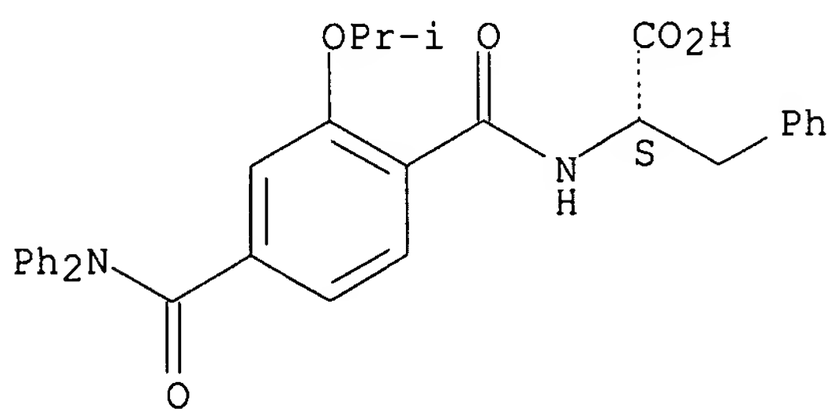
RN 852065-36-2 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 852065-37-3 CAPLUS
CN L-Phenylalanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:362563 CAPLUS
DN 141:98999
TI Novel factor Xa inhibitors based on a benzoic acid scaffold and incorporating a neutral P1 ligand
AU Nazare, Marc; Matter, Hans; Klingler, Otmar; Al-Obeidi, Fahad; Schreuder, Herman; Zoller, Gerhard; Czech, Jorg; Lorenz, Martin; Dudda, Angela; Peyman, Anusch; Nestler, Hans Peter; Urmann, Matthias; Bauer, Armin; Laux, Volker; Wehner, Volkmar; Will, David W.
CS Aventis Pharma Deutschland GmbH, Frankfurt, D-65926, Germany
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(11), 2801-2805
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 141:98999
GI

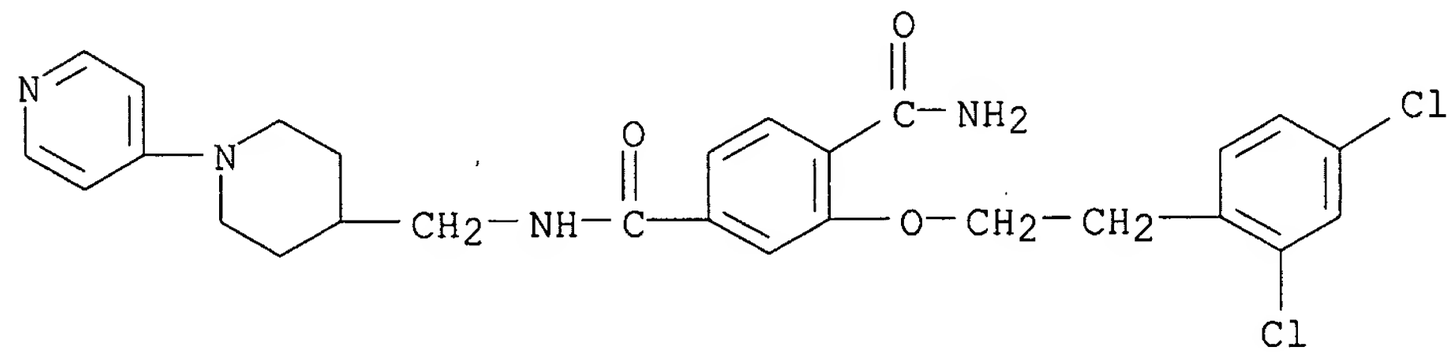
I

AB A series of novel, highly potent, achiral factor Xa inhibitors based on a benzoic acid scaffold and containing a chlorophenethyl moiety directed towards the protease S1 pocket is described. A number of structural features, such as the requirements of the P1, P4 and ester-binding pocket ligands were explored with respect to inhibition of factor Xa. Compound (I) was the most potent compound in a series of antithrombotic secondary assays.

IT 717902-18-6
RL: PAC (Pharmacological activity); BIOL (Biological study)
(novel factor Xa inhibitors based on a benzoic acid scaffold and incorporating a neutral P1 ligand)

RN 717902-18-6 CAPLUS

CN 1,4-Benzenedicarboxamide, 2-[2-(2,4-dichlorophenyl)ethoxy]-N4-[[1-(4-pyridinyl)-4-piperidinyl]methyl]- (CA INDEX NAME)



RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:189140 CAPLUS
DN 140:350050
TI Terephthalamide derivatives as mimetics of the helical region of Bak peptide target Bcl-xL protein
AU Yin, Hang; Hamilton, Andrew D.
CS Department of Chemistry, Yale University, New Haven, CT, 06511, USA
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(6), 1375-1379
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 140:350050

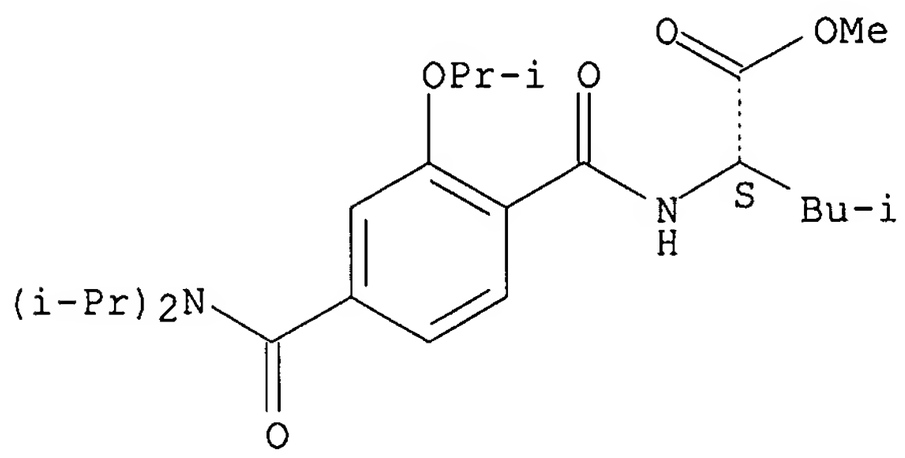
AB A group of novel Bcl-xL/Bak antagonists, based on a terephthalamide scaffold, were designed to mimic the α-helical region of the Bak peptide. Good in vitro inhibition potencies in disrupting the Bak/Bcl-xL complex have been observed (terephthalamide 4, Ki=0.78±0.07 μM).

IT 681465-54-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)

RN 681465-54-3 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

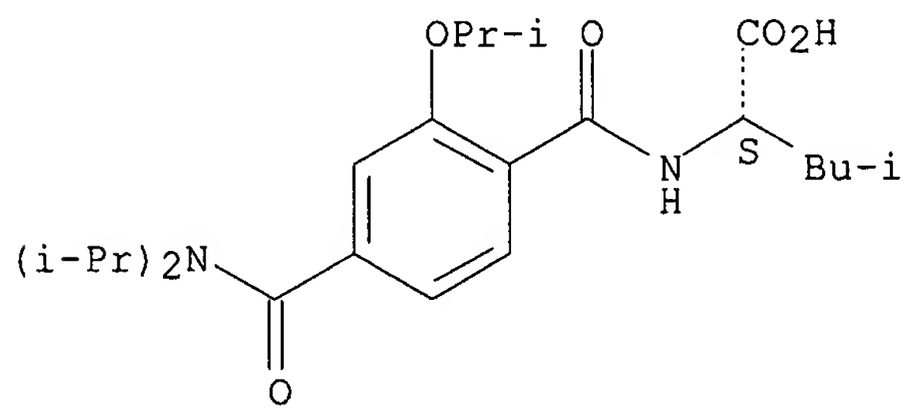


IT 681465-56-5P 681465-58-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)

RN 681465-56-5 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

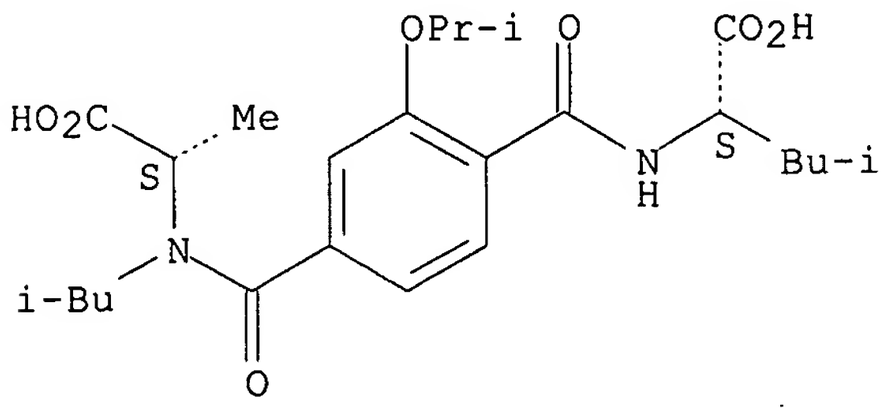
Absolute stereochemistry.



RN 681465-58-7 CAPLUS

CN L-Leucine, N-[4-[[[(1S)-1-carboxyethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

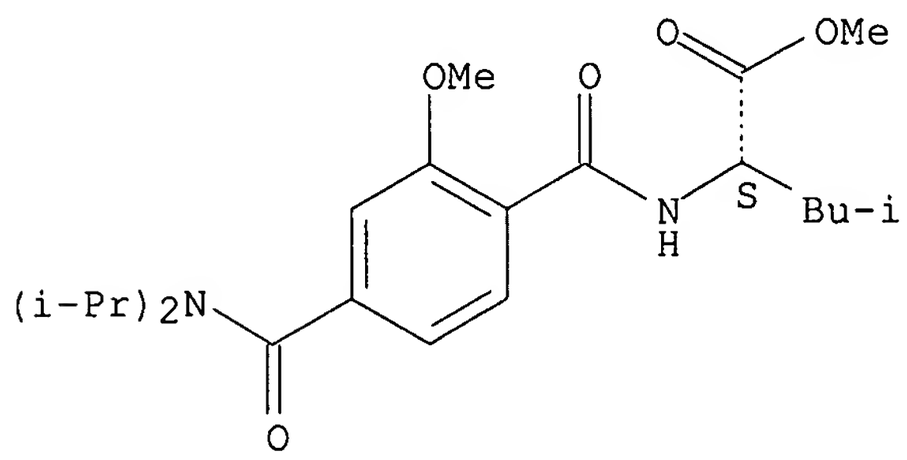
Absolute stereochemistry. Rotation (-).



IT 681465-60-1 681465-62-3 681465-68-9
681465-70-3 681465-72-5 681465-74-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)

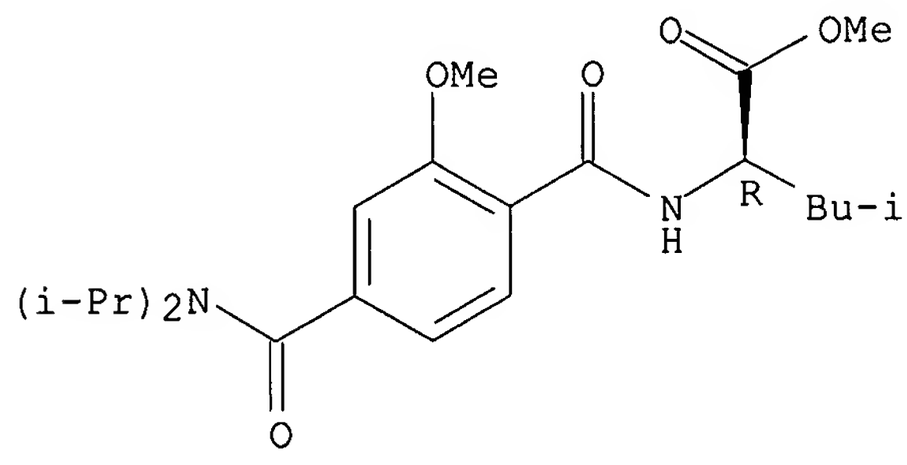
RN 681465-60-1 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



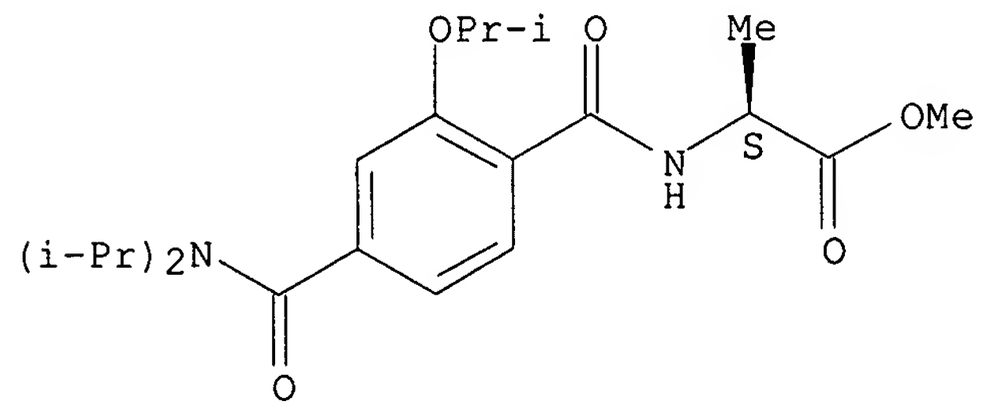
RN 681465-62-3 CAPLUS
CN D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



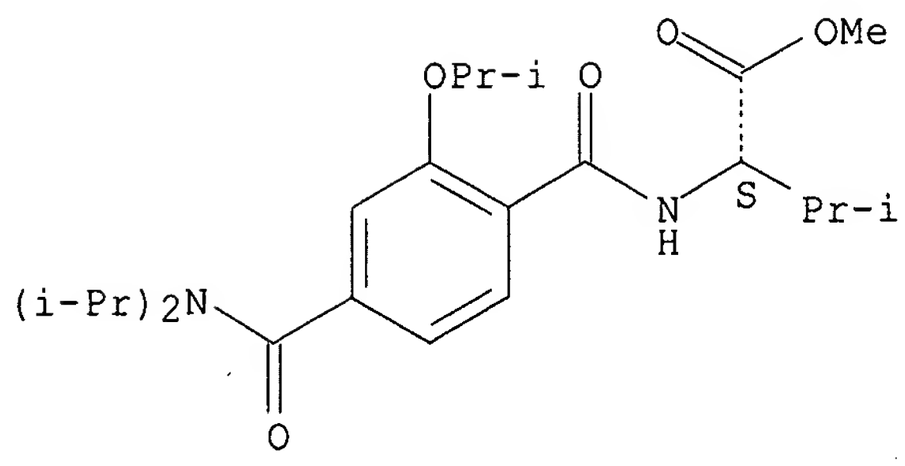
RN 681465-68-9 CAPLUS
CN L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



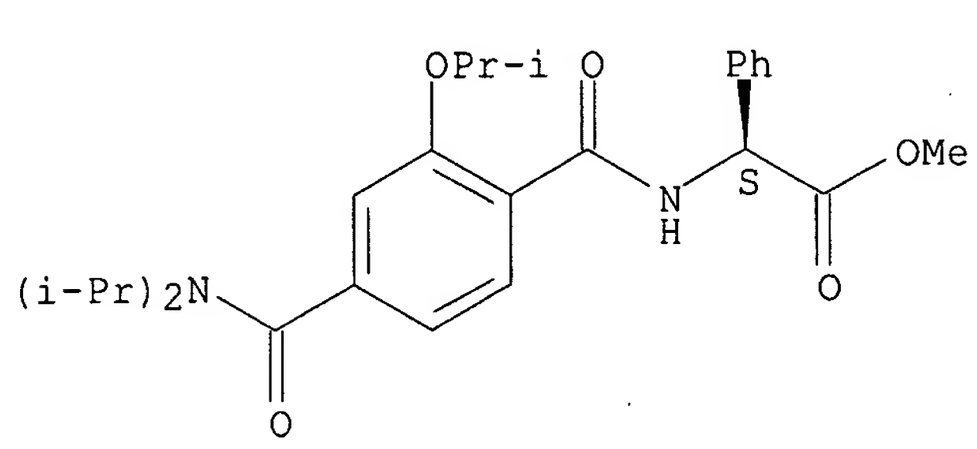
RN 681465-70-3 CAPLUS
CN L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



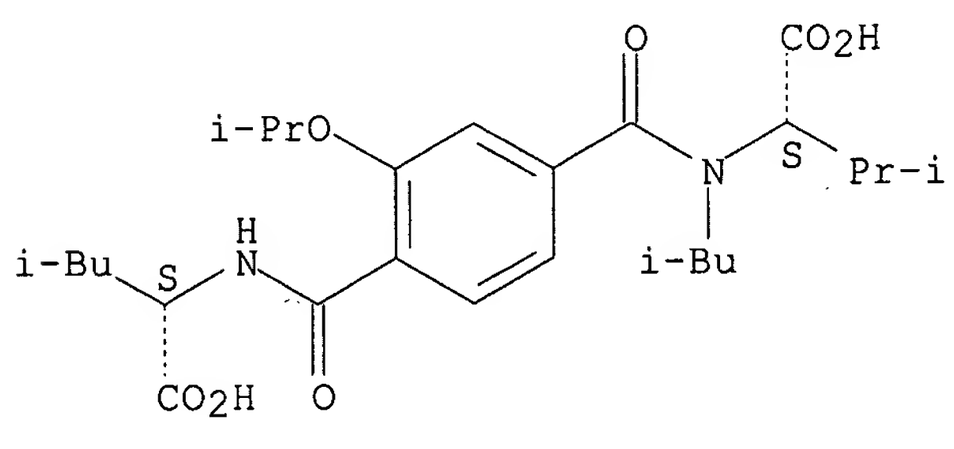
RN 681465-72-5 CAPLUS
CN Benzeneacetic acid, α-[[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



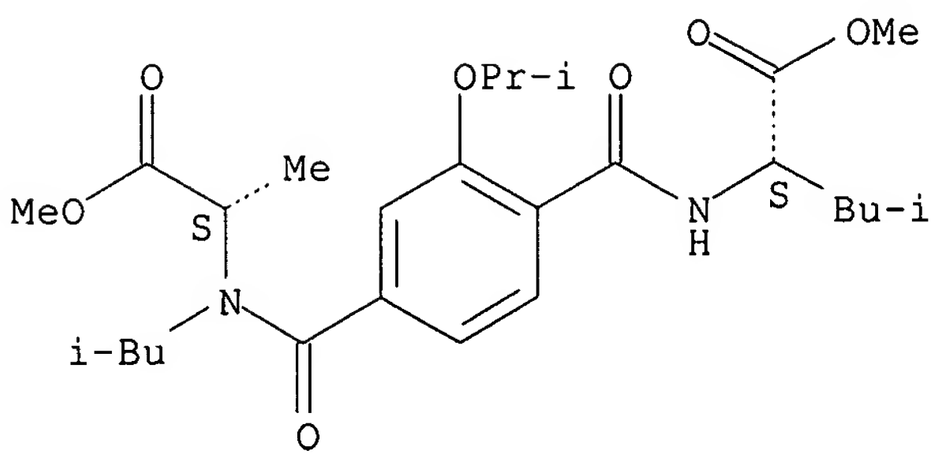
RN 681465-74-7 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 681466-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)
RN 681466-00-2 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-2-methoxy-1-methyl-2-oxoethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:991333 CAPLUS
DN 140:35967
TI Methods of treating Alzheimers disease using aromatically substituted ω-amino-alkanoic acid amides and alkanoic acid diamides
IN Maillard, Michel; Varghese, John
PA Elan Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 286 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003103652	A1	20031218	WO 2003-US18283	20030611
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2003237546	A1	20031222	AU 2003-237546	20030611
	US 2006089355	A1	20060427	US 2005-517981	20050714
PRAI	US 2002-387756P	P	20020611		
	WO 2003-US18283	W	20030611		

OS MARPAT 140:35967

AB Disclosed are methods for treating Alzheimer's disease (no data), and other diseases (no data), and/or inhibiting beta-secretase enzyme (no data), and/or inhibiting deposition of amyloid β peptide (no data) in a mammal, using ω-amino-alkanoic acid amides and alkanoic acid diamides (R1-X1-NH-X2-CH(R2)CH2CH(R3)CH(OH)CH2CH(R4)C(O)NH-R5 (I); variables defined below; e.g. (2S,4S,5S,7R)-N-(4-amino-7-butyl-7-carbamoyl-5-hydroxy-2-isopropyloctyl)-3-methoxy-2-(3-methoxypropoxy)benzamide). Many example prepns. are included but all of them comprise an English translation of a German patent (EP 0716077 A1; 1996; CA file accession number 125:167576). For I: R1 is a 2-RA-3-RB-Ph radical, a 2-RA-4-Rc-Ph radical, a 2-RA-pyridin-3-yl radical a 3-RA-pyridin-2-yl radical or a 1-RD-indol-3-yl radical, wherein one of the radicals RA and RB is an aliphatic or heterocycloaliph.-aliphatic radical or free or aliphatically, araliphatically or heteroaraliphatically etherified hydroxy and the other is H, an aliphatic radical or free or esterified or amidated carboxy, RC is H, an aliphatic radical, free or aliphatically, araliphatically, heteroaraliphatically or heteroarylaliphatically etherified hydroxy or an unsubstituted or heteroaliphatically substituted amino group, and RD is an aliphatic, araliph. or heteroaliph. radical, one of the radicals X1 and X2 is

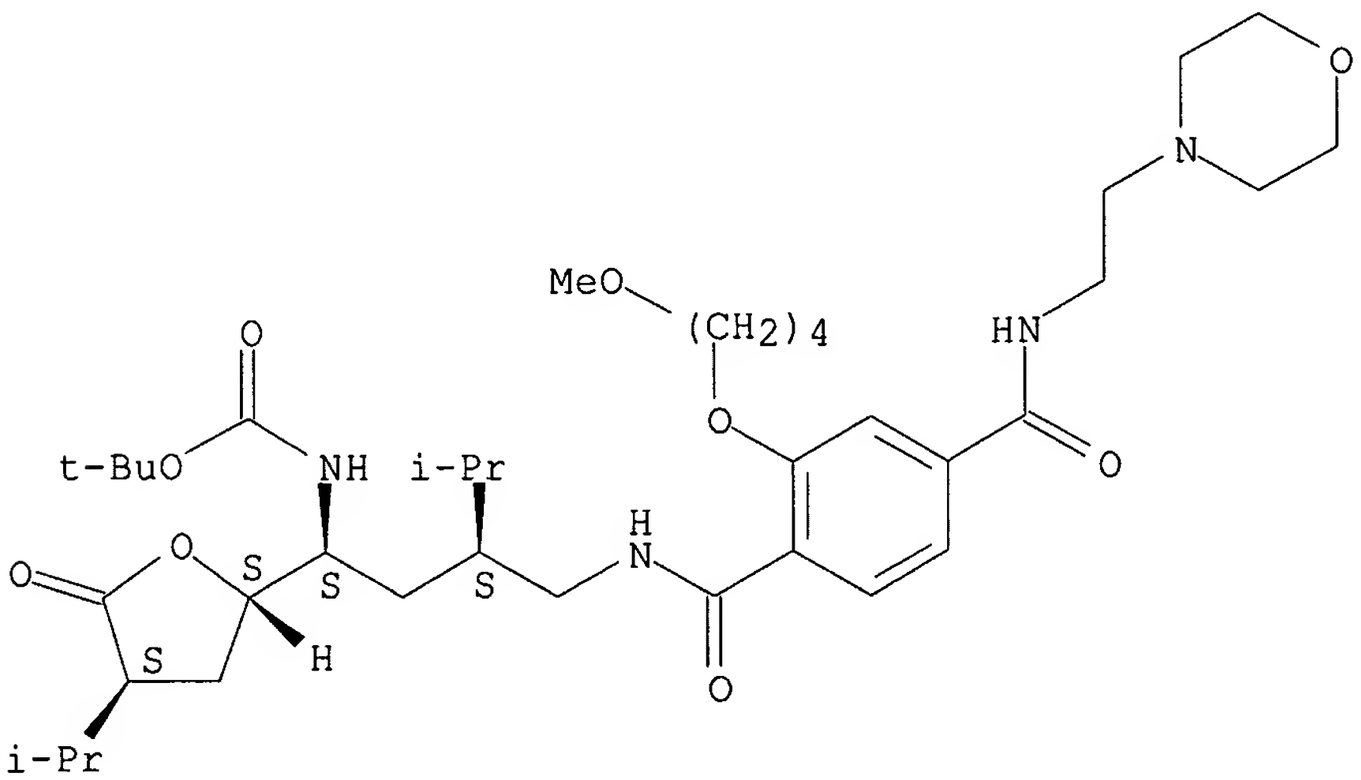
carbonyl and the other is methylene, R2 is an aliphatic radical, R3 is unsubstituted or aliphatically substituted amino, R4 is an aliphatic or araliph. radical, and R5 is an aliphatic or cycloaliph.-aliphatic radical or an optionally hydrogenated and/or oxo-substituted heteroaryl radical or an optionally hydrogenated and/or oxo-substituted heteroaryl or heteroaliph. radical bonded via a C atom.

IT 179995-21-2P 179995-22-3P 179995-71-2P
179995-72-3P 179995-73-4P 179995-74-5P
179995-97-2P 179996-13-5P 180183-42-0P
180183-63-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; methods of treating Alzheimers disease using aromatically substituted ω-amino-alkanoic acid amides and alkanoic acid diamides)

RN 179995-21-2 CAPLUS

CN Carbamic acid, [(1S,3S)-3-[[[2-(4-methoxybutoxy)-4-[[[2-(4-morpholinyl)ethyl]amino]carbonyl]benzoyl]amino]methyl]-4-methyl-1-[(2S,4S)-tetrahydro-4-(1-methylethyl)-5-oxo-2-furanyl]pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

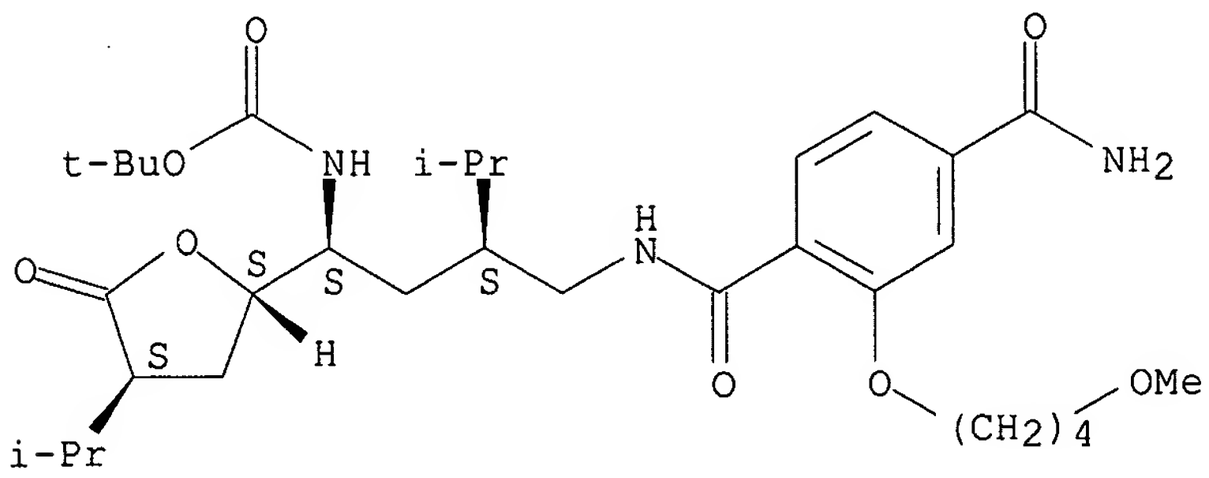
Absolute stereochemistry.



RN 179995-22-3 CAPLUS

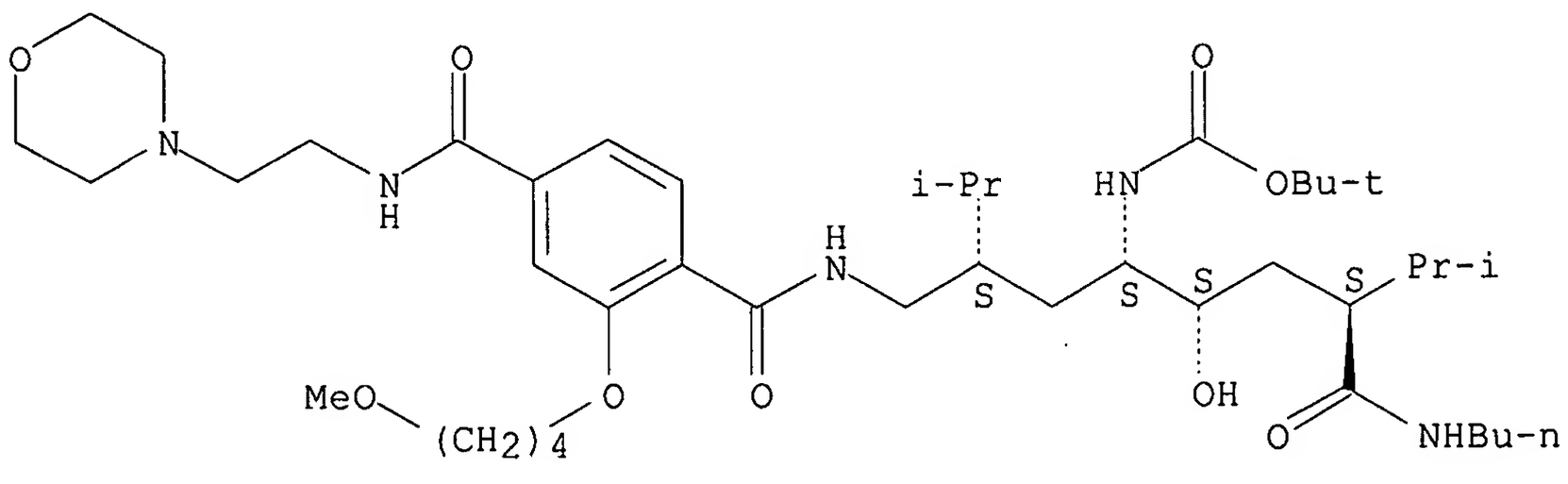
CN Carbamic acid, [(1S,3S)-3-[[[4-(aminocarbonyl)-2-(4-methoxybutoxy)benzoyl]amino]methyl]-4-methyl-1-[(2S,4S)-tetrahydro-4-(1-methylethyl)-5-oxo-2-furanyl]pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



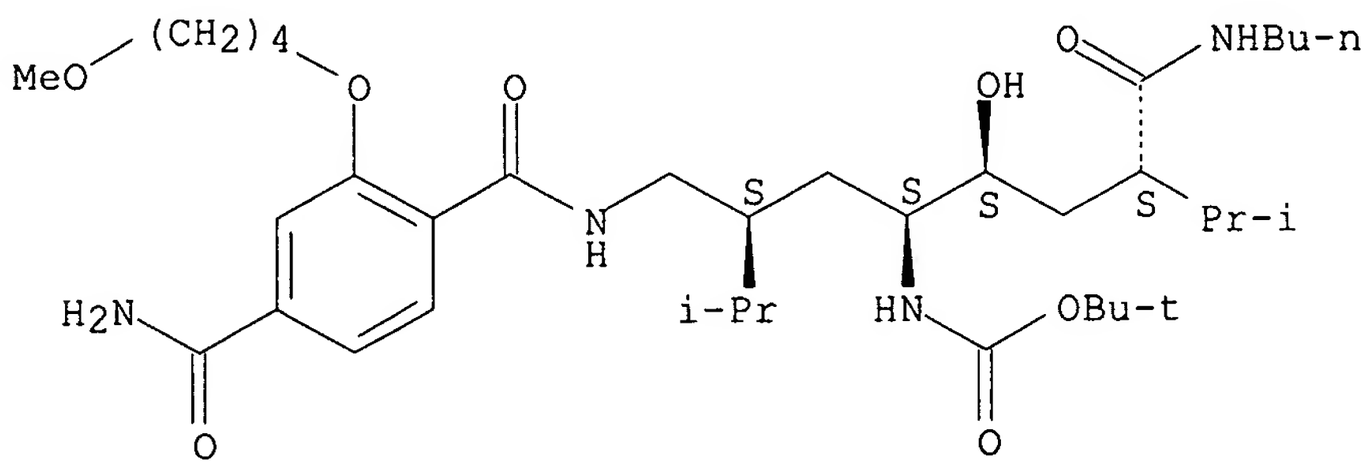
RN 179995-71-2 CAPLUS
CN Carbamic acid, [(1S,2S,4S)-4-[(butylamino)carbonyl]-2-hydroxy-1-[(2S)-2-[[[2-(4-methoxybutoxy)-4-[[[2-(4-morpholinyl)ethyl]amino]carbonyl]benzoyl]amino]methyl]-3-methylbutyl]-5-methylhexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



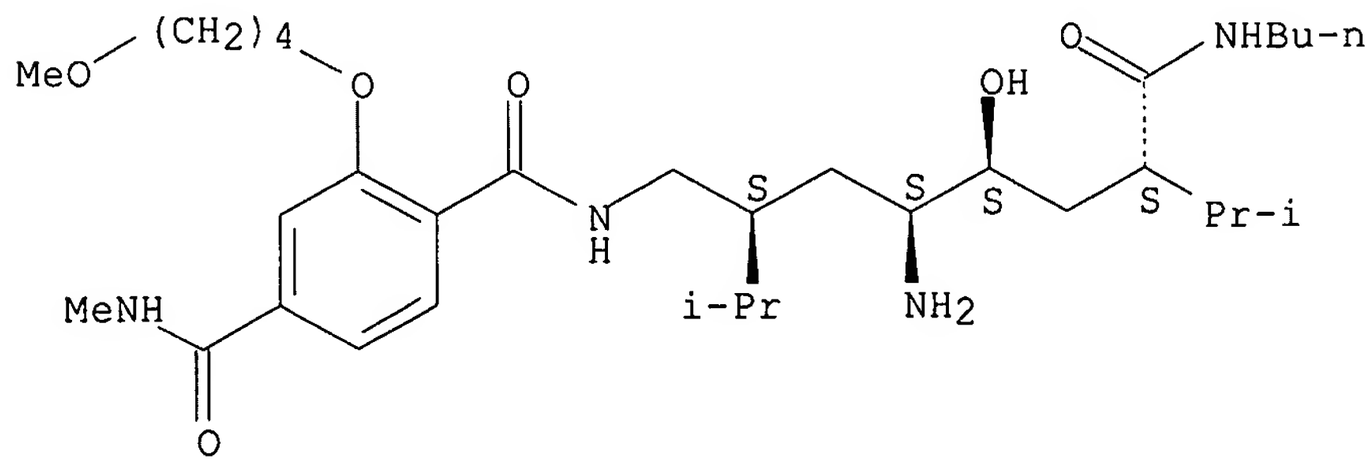
RN 179995-72-3 CAPLUS
CN Carbamic acid, [(1S,2S,4S)-1-[(2S)-2-[[[4-(aminocarbonyl)-2-(4-methoxybutoxy)benzoyl]amino]methyl]-3-methylbutyl]-4-[(butylamino)carbonyl]-2-hydroxy-5-methylhexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 179995-73-4 CAPLUS
CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-[(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-methoxybutoxy)-N4-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

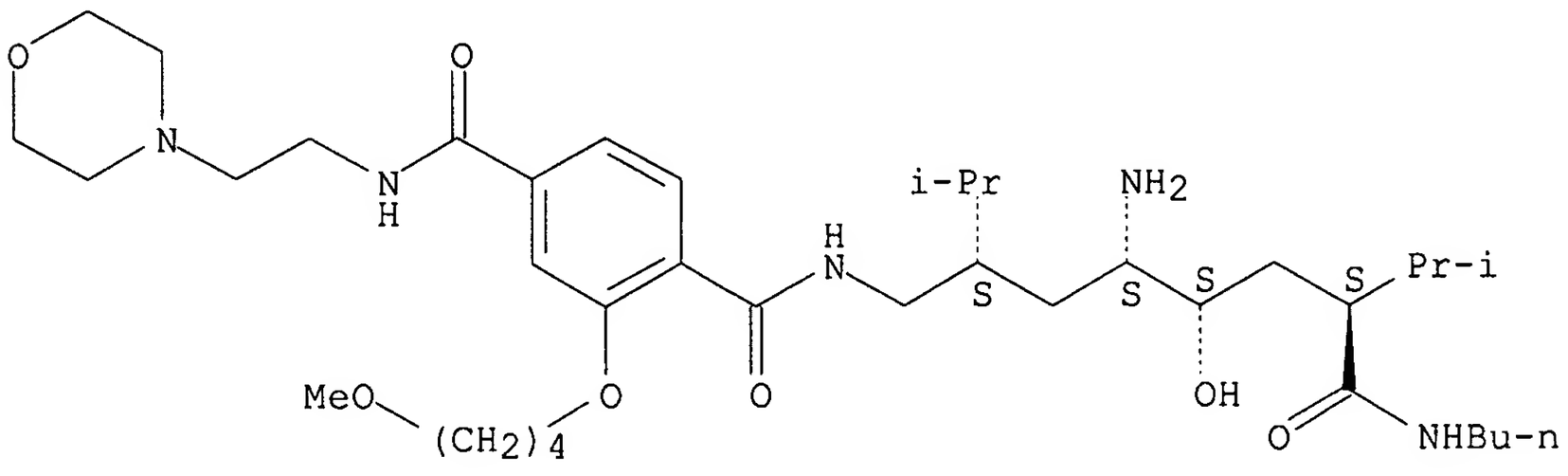
Absolute stereochemistry.



● HCl

RN 179995-74-5 CAPLUS
CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-[(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-methoxybutoxy)-N4-[2-(4-morpholinyl)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

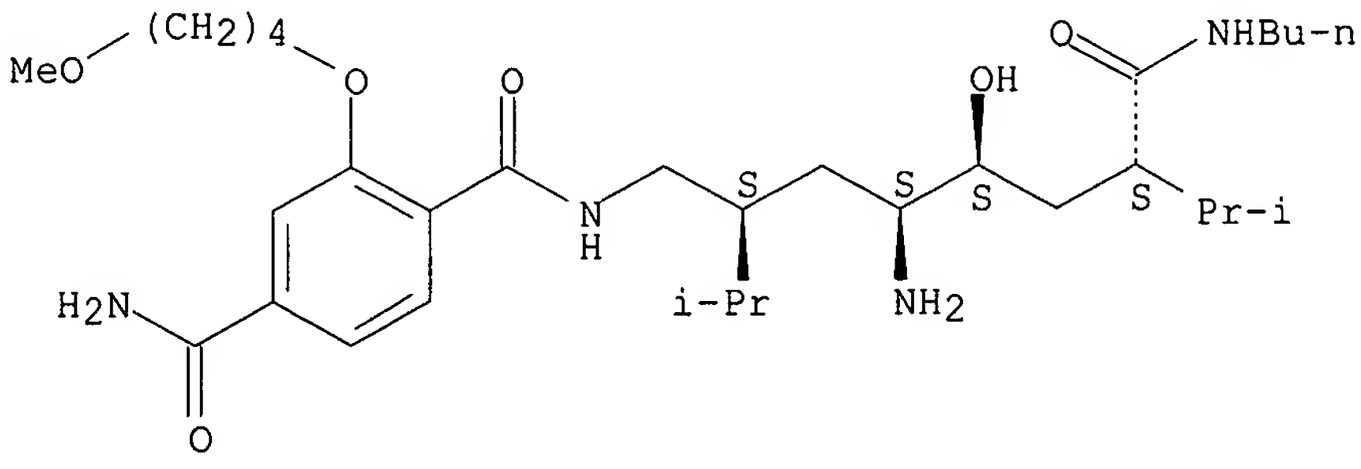
Absolute stereochemistry.



● HCl

RN 179995-97-2 CAPLUS
CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-[(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-methoxybutoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

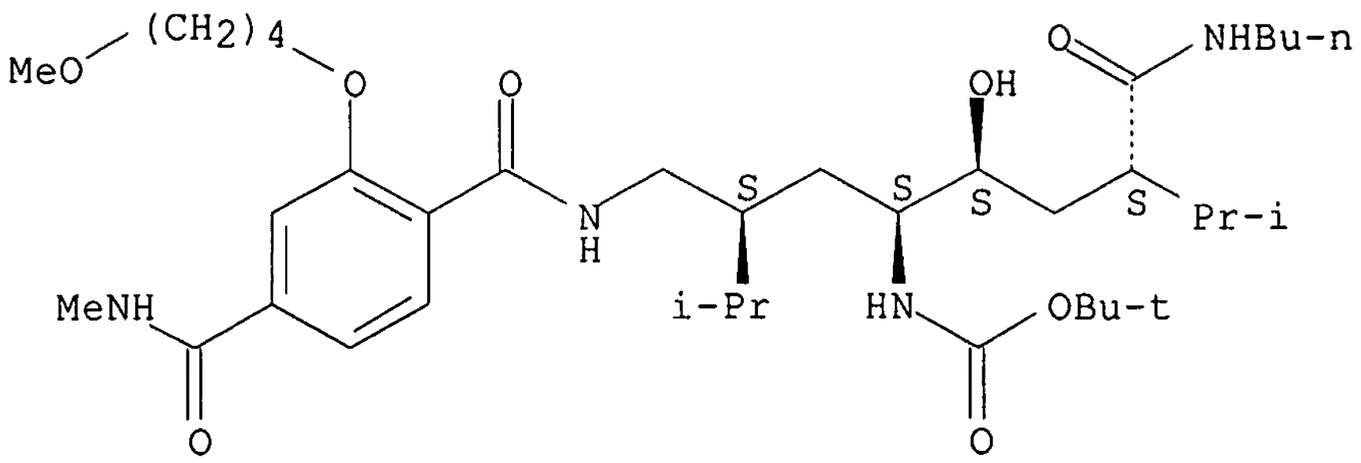
Absolute stereochemistry.



● HCl

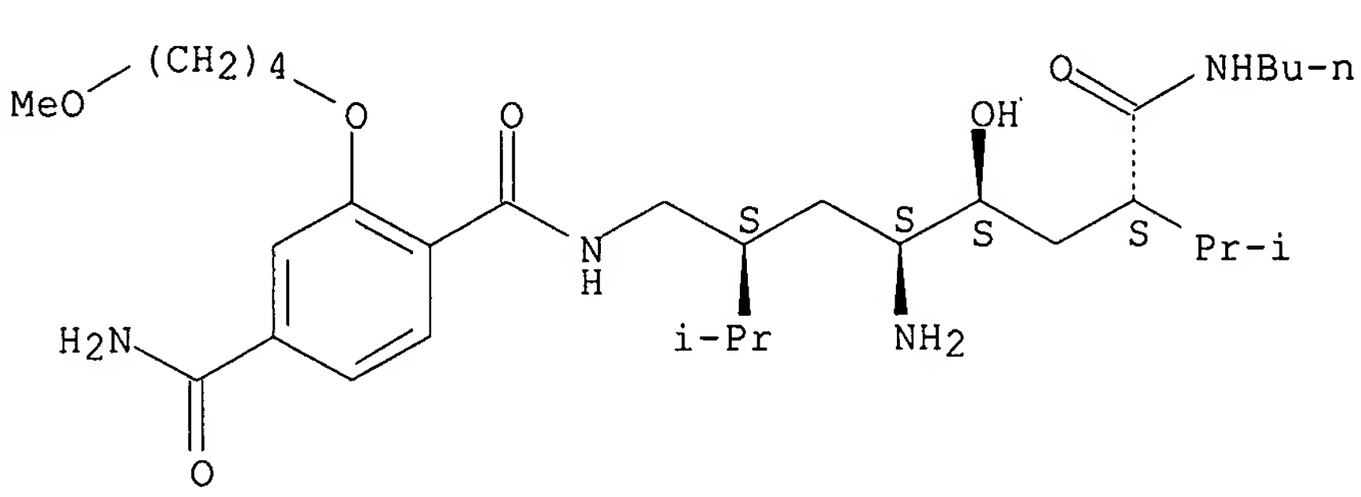
RN 179996-13-5 CAPLUS
CN Carbamic acid, [(1S,2S,4S)-4-[(butylamino)carbonyl]-2-hydroxy-1-[(2S)-2-[[[2-(4-methoxybutoxy)-4-[(methylamino)carbonyl]benzoyl]amino]methyl]-3-methylbutyl]-5-methylhexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



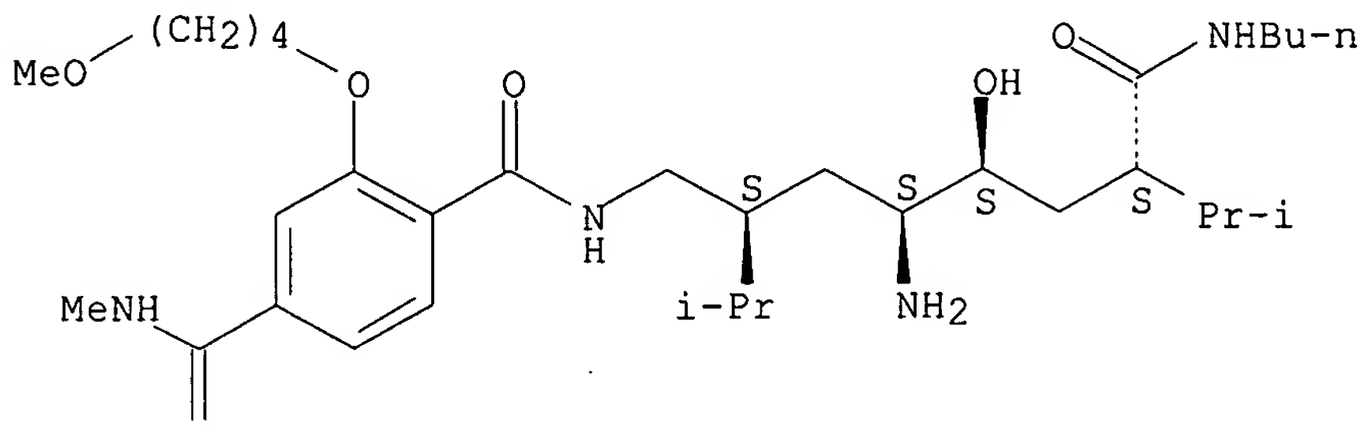
RN 180183-42-0 CAPLUS
CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-[(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-methoxybutoxy)- (CA INDEX NAME)

Absolute stereochemistry.



RN 180183-63-5 CAPLUS
CN 1,4-Benzenedicarboxamide, N1-[(2S,4S,5S,7S)-4-amino-7-[(butylamino)carbonyl]-5-hydroxy-8-methyl-2-(1-methylethyl)nonyl]-2-(4-methoxybutoxy)-N4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:952818 CAPLUS
DN 140:146599
TI Unsaturated alkoxy-substituted poly(p-phenylene 1,3,4-oxadiazole)s: Synthesis and chemical-physical characterization
AU Capitani, Donatella; Laurienzo, Paola; Malinconico, Mario; Proietti, Noemi; Roviello, Antonio
CS Istituto di Metodologie Chimiche, C.N.R., Monterotondo Stazione, 00016, Italy
SO Journal of Polymer Science, Part A: Polymer Chemistry (2003), 41(24), 3916-3928

CODEN: JPACEC; ISSN: 0887-624X
PB John Wiley & Sons, Inc.
DT Journal
LA English
AB A new series of alkoxy-substituted poly(p-phenylene 1,3,4-oxadiazole)s modified by the insertion of small percentages of various comonomers were synthesized through the precursor polyhydrazides. The comonomers used contained trans double bonds or meta-alkoxy-substituted aromatic rings to improve the solubility of the final polymers. The synthesized copolymers were chemical characterized by 1H NMR and Fourier transform IR spectroscopy. In some cases, the copolymers really showed improved solubility in organic solvents.

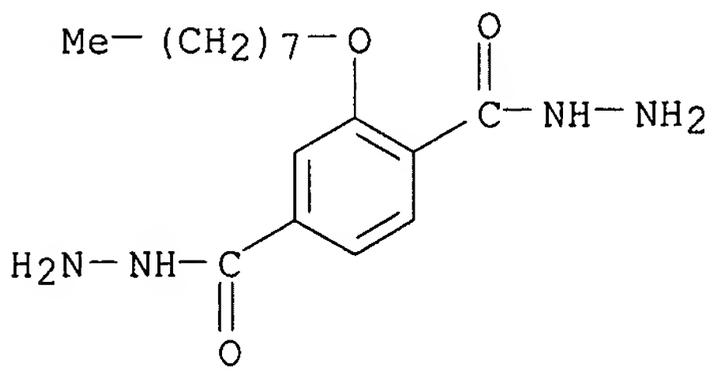
The 15N solid-state NMR technique was applied to examine the degree of conversion from the precursor polyhydrazides to the final polymers, which determined the effective conjugated length in the target polyoxadiazoles. Thermal stability and structural characteristics of all the polymers as well as a preliminary investigation on the optical properties of polyoxadiazoles are also reported. The copolymers retained high absorbance in the UV region and high transmission in the whole telecommunication range.

IT 428516-44-3P 651054-59-0P 651054-60-3P
651054-61-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(precursor; synthesis and chemical-phys. characterization of unsatd. alkoxy-substituted poly(phenylene oxadiazole)s)

RN 428516-44-3 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with 2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

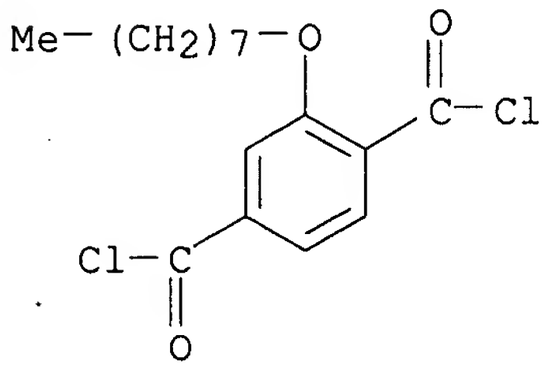
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



CM 2

CRN 321588-70-9
CMF C16 H20 Cl2 O3

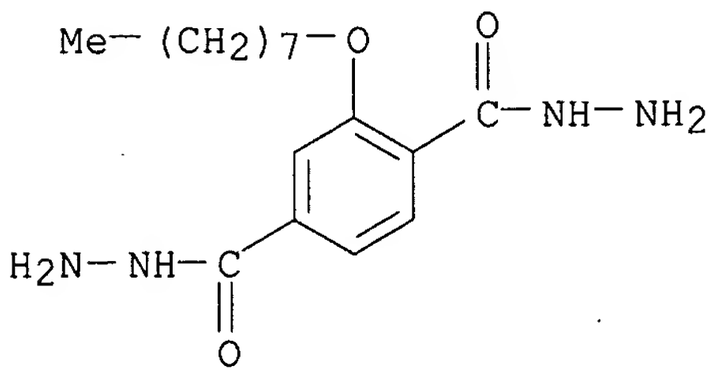


RN 651054-59-0 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-butenedioyl dichloride and 2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

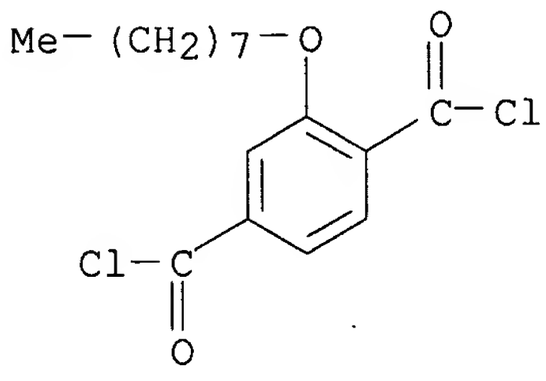
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



CM 2

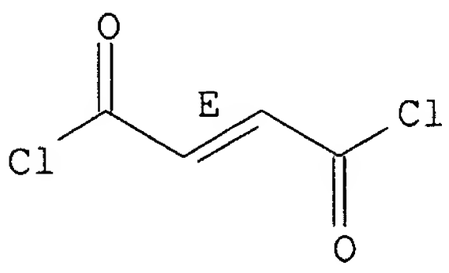
CRN 321588-70-9
CMF C16 H20 Cl2 O3



CM 3

CRN 627-63-4
CMF C4 H2 Cl2 O2

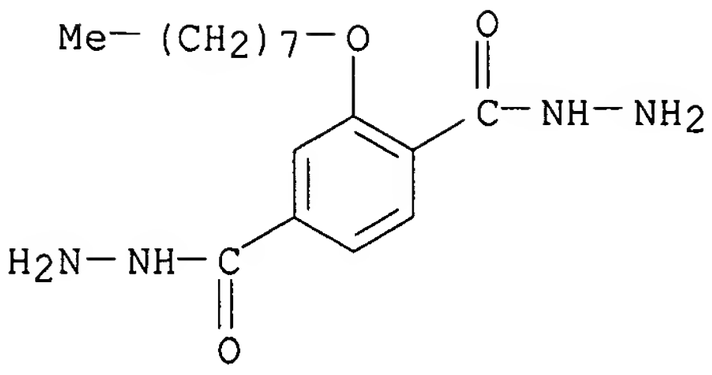
Double bond geometry as shown.



RN 651054-60-3 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-methyl-2-butenedioyl dichloride and 2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

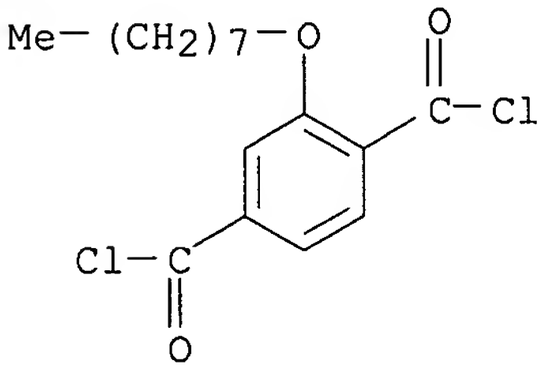
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



CM 2

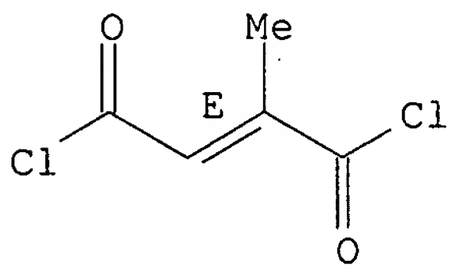
CRN 321588-70-9
CMF C16 H20 C12 O3



CM 3

CRN 20537-97-7
CMF C5 H4 C12 O2

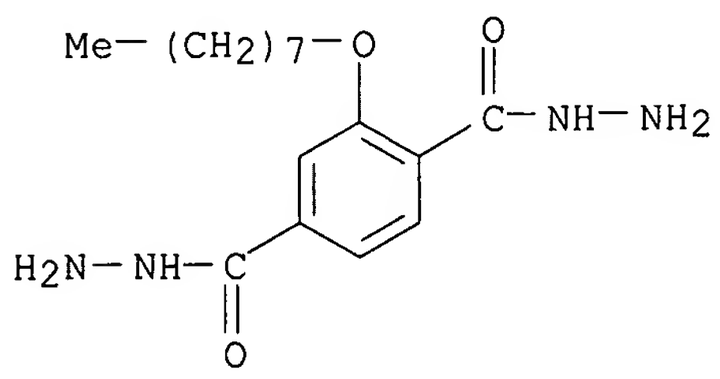
Double bond geometry as shown.



RN 651054-61-4 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-methyl-2-butenedioyl dichloride, 2-(octyloxy)-1,4-benzenedicarbonyl dichloride and 4-(octyloxy)-1,3-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

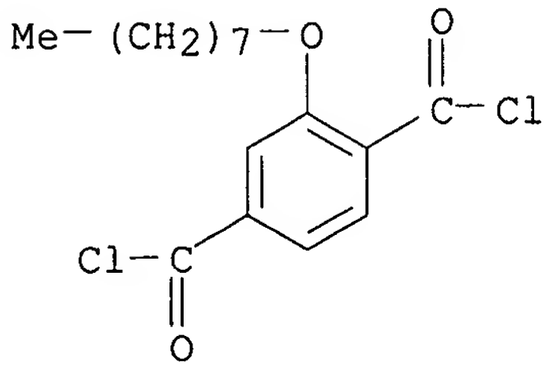
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



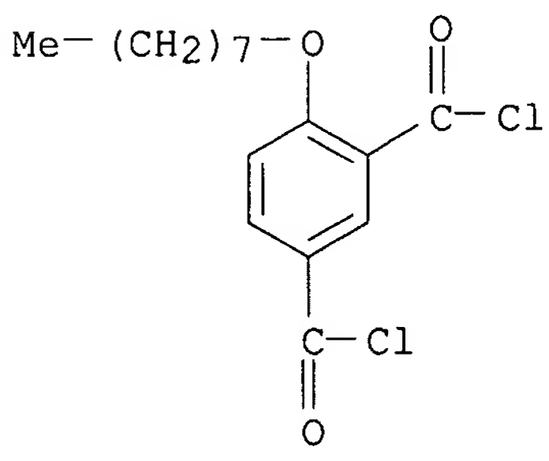
CM 2

CRN 321588-70-9
CMF C16 H20 Cl2 O3



CM 3

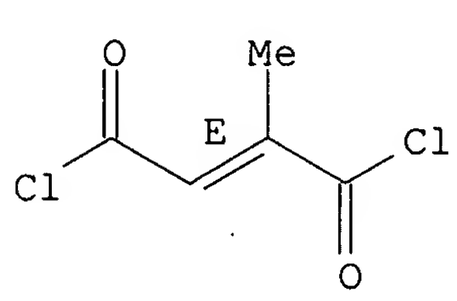
CRN 70065-39-3
CMF C16 H20 Cl2 O3



CM 4

CRN 20537-97-7
CMF C5 H4 Cl2 O2

Double bond geometry as shown.

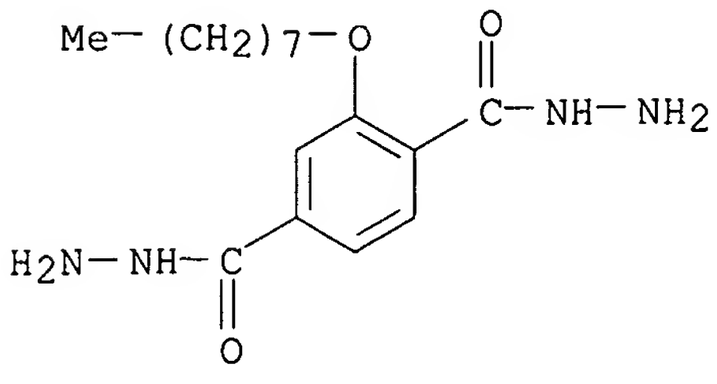


IT 651054-59-0DP, cyclodehydrated 651054-60-3DP, cyclodehydrated 651054-61-4DP, cyclodehydrated
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and chemical-phys. characterization of unsatd. alkoxy-substituted poly(phenylene oxadiazole)s)

RN 651054-59-0 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-butenedioyl dichloride and 2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

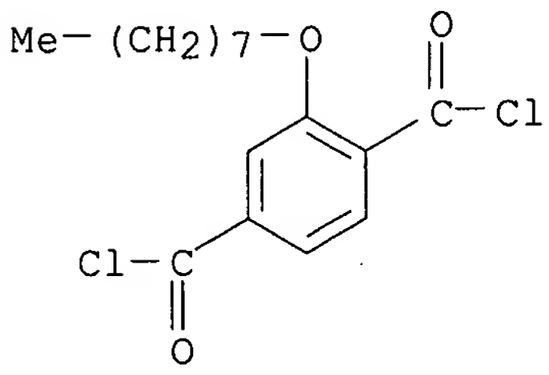
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



CM 2

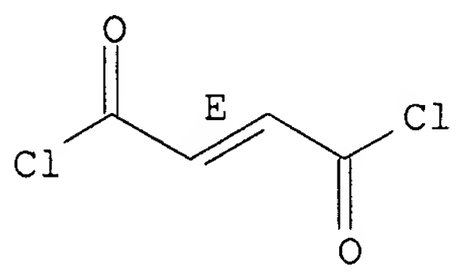
CRN 321588-70-9
CMF C16 H20 Cl2 O3



CM 3

CRN 627-63-4
CMF C4 H2 Cl2 O2

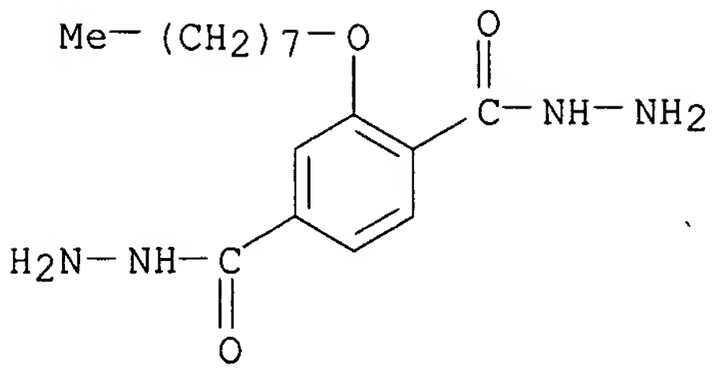
Double bond geometry as shown.



RN 651054-60-3 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-methyl-2-butenedioyl dichloride and 2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

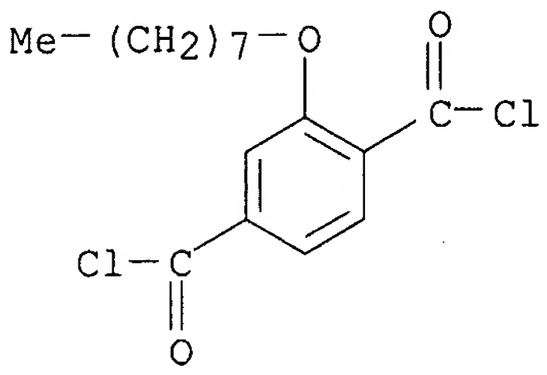
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



CM 2

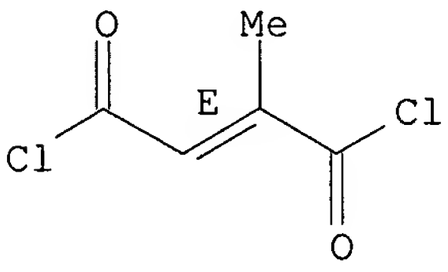
CRN 321588-70-9
CMF C16 H20 C12 O3



CM 3

CRN 20537-97-7
CMF C5 H4 C12 O2

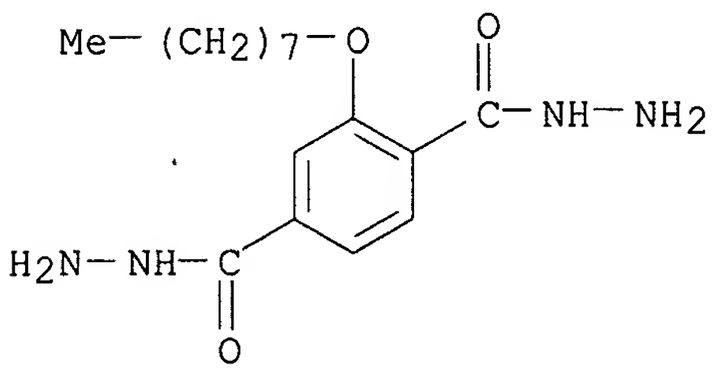
Double bond geometry as shown.



RN 651054-61-4 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with (2E)-2-methyl-2-butenedioyl dichloride, 2-(octyloxy)-1,4-benzenedicarbonyl dichloride and 4-(octyloxy)-1,3-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

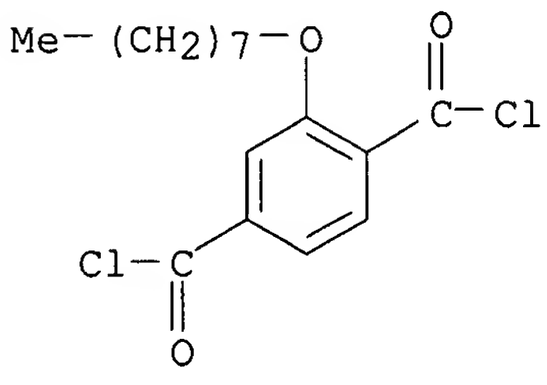
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



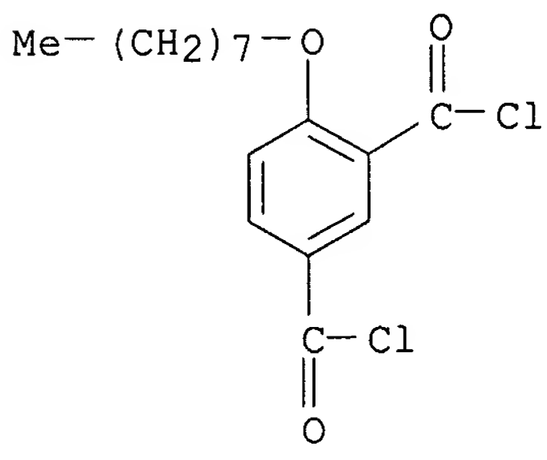
CM 2

CRN 321588-70-9
CMF C16 H20 Cl2 O3



CM 3

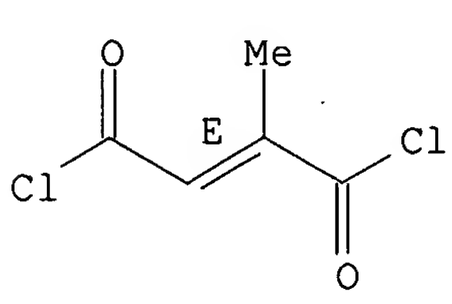
CRN 70065-39-3
CMF C16 H20 Cl2 O3



CM 4

CRN 20537-97-7
CMF C5 H4 Cl2 O2

Double bond geometry as shown.



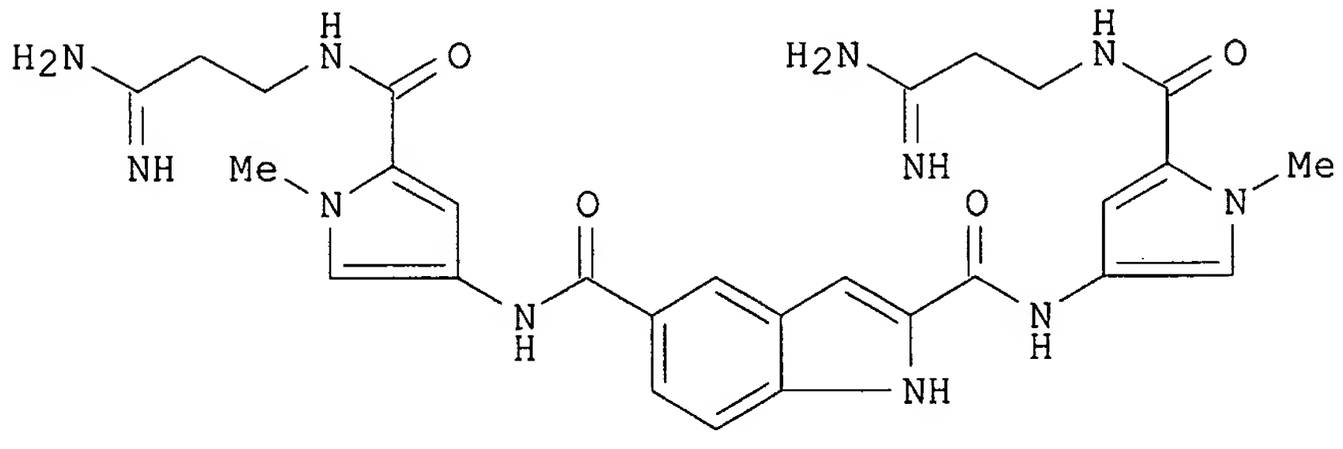
RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:551374 CAPLUS
DN 139:117331
TI Preparation of polyamide analogs possessing antibacterial, antifungal, and/or antitumor activity
IN Dyatkina, Natalia B.; Shi, Dong-fang; Roberts, Christopher Don; Velligan, Mark Douglas; Liehr, Sebastian Johannes Reinhard; Botyanszki, Janos; Zhang, Wentao; Khorlin, Alexander; Nelson, Peter Harold; Muchowski, Joseph Martin

PA Genelabs Technologies, Inc., USA; et al.
SO PCT Int. Appl., 174 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003057212	A1	20030717	WO 2002-US41087	20021224
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002364209	A1	20030724	AU 2002-364209	20021224
	US 2003212113	A1	20031113	US 2002-328710	20021224
	US 7064218	B2	20060620		
	BR 2002007583	A	20040427	BR 2002-7583	20021224
	NO 2003003773	A	20031023	NO 2003-3773	20030825
PRAI	US 2001-343796P	P	20011226		
	US 2001-343829P	P	20011226		
	WO 2002-US41087	W	20021224		

OS MARPAT 139:117331
GI



I

AB Compds. of formula R1Z1COX1NHCOX2CONHX3COZ2R2 [wherein Z1 and Z2 = independently NR3, O; R3 = H, alkyl; R1 and R2 = independently substituted alkyl or aryl, (un)substituted heteroaryl; X2 = (un)substituted aryl or heteroaryl, alkenyl, alkynyl, cycloalkyl, heterocyclic; X1 and X3 = independently (un)substituted aryl or heteroaryl, CHR4; R4 = (un)natural amino acid side chain; or their pharmaceutically acceptable salts] were prepared as topoisomerase inhibitors (no data) for use as antibacterial, antifungal, and/or antitumor agents. For example, 1H-indole-2,5-dicarboxylic acid dipentafluorophenyl ester was reacted with at least two equivalent of 4-amino-1-methyl-1H-pyrrole-2-carboxylic acid [2-(carbamimidoyl)ethyl]amide in DMF to give I. Compds. of the invention exhibited antibacterial and antifungal activity with some having minimal inhibitory concns. of <45.5 μM. DNA binding assays showed that invention compds. bind to DNA very tightly, with apparent Kd,app values below 100 nM for most compds. tested.

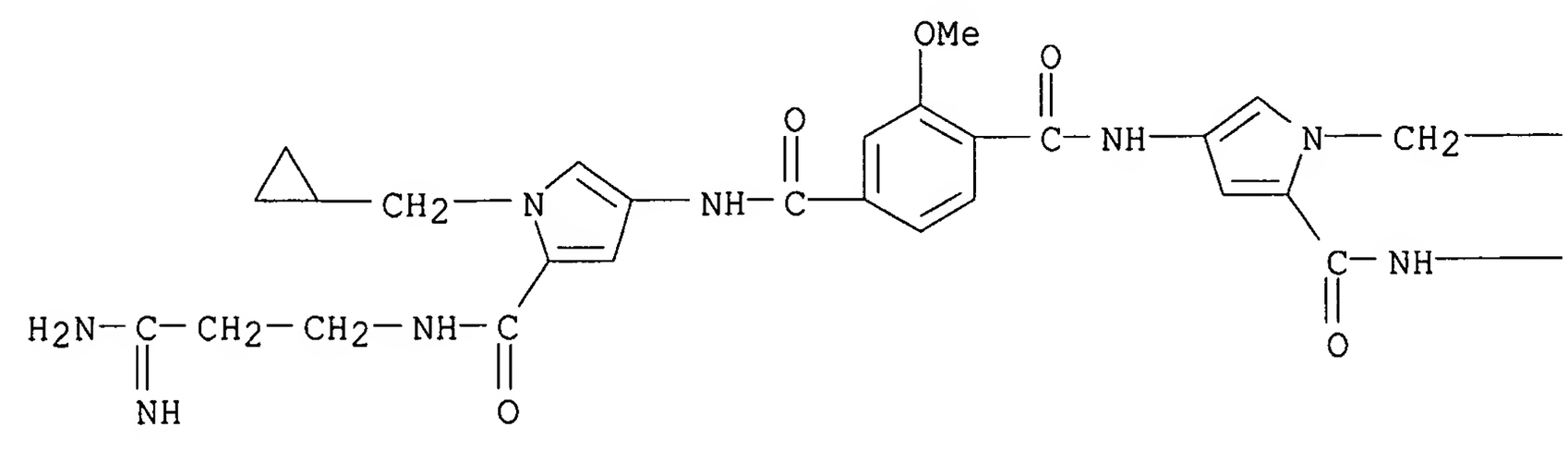
IT 386253-05-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(drug candidate; preparation of polyamides as antibacterial, antifungal, and/or antitumor agents)

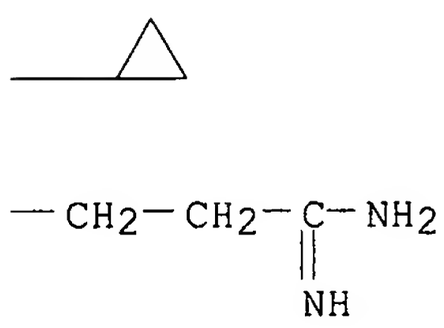
RN 386253-05-0 CAPLUS

CN 1,4-Benzenedicarboxamide, N,N'-bis[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-(cyclopropylmethyl)-1H-pyrrol-3-yl]-2-methoxy- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:881449 CAPLUS

DN 138:145393

TI Synthesis and liquid crystalline properties of low molecular mass compounds containing the 1,4-bis(5-phenyl-1,3,4-oxadiazolyl)benzene unit

AU Acierno, Domenico; Concilio, Simona; Diodati, Angela; Iannelli, Pio; Piotto, Stefano P.; Scarfato, Paola

CS Dipartimento di Ingegneria dei Materiali e della Produzione, Universita di Napoli, Naples, I-80125, Italy

SO Liquid Crystals (2002), 29(11), 1383-1392
CODEN: LICRE6; ISSN: 0267-8292

PB Taylor & Francis Ltd.

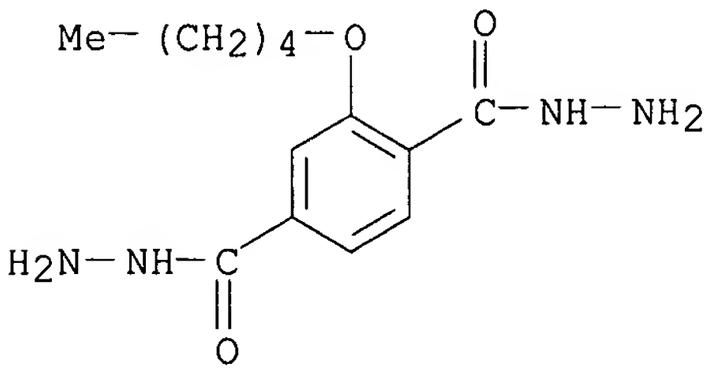
DT Journal

LA English

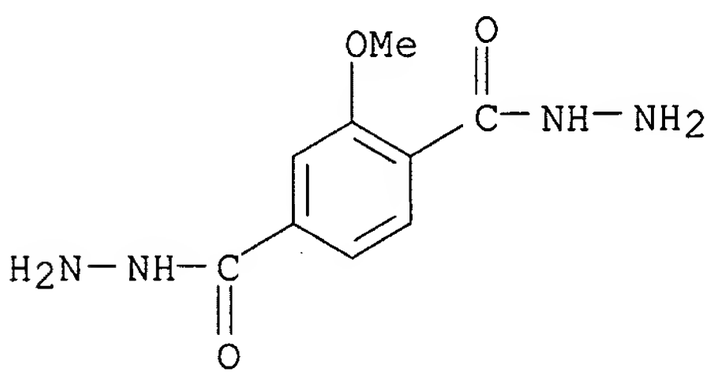
AB The synthesis and characterization of low mol. mass compds. containing 1,4-bis(5-phenyl-1,3,4-oxadiazolyl)benzene is reported. All compds. are fluorescent in solution Due to the flat shape of the conjugated unit, smectic-like packing is observed at high temps. for some of the synthesized compds. Also the insertion of a lateral flexible alkoxy unit strongly destabilizes the smectic order while promoting the appearance of a nematic phase in the case of the shortest methoxy unit. The mesogenic character of this unit may be of interest in the synthesis of liquid crystalline polymeric systems, taking advantage of both the fluorescent properties and the peculiar mol. structure of the liquid crystalline state.

IT 428516-39-6P, Pentyloxyterephthalic dihydrazide
492458-31-8P, Methoxyterephthalic dihydrazide 492458-32-9P
, Nonyloxyterephthalic dihydrazide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and esterification of)

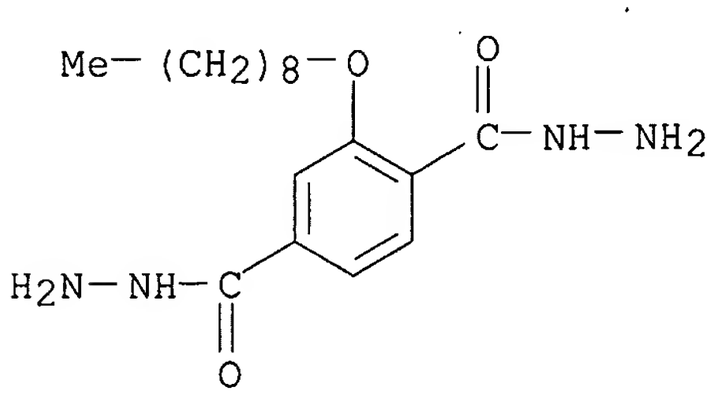
RN 428516-39-6 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(pentyloxy)-, dihydrazide (9CI) (CA INDEX
NAME)



RN 492458-31-8 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-methoxy-, dihydrazide (9CI) (CA INDEX
NAME)



RN 492458-32-9 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(nonyloxy)-, dihydrazide (9CI) (CA INDEX
NAME)



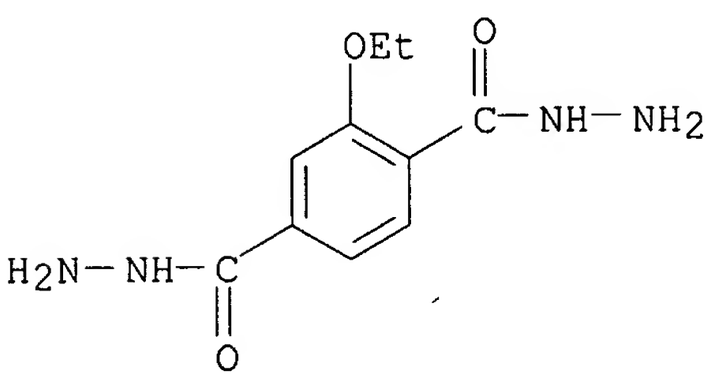
RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:234092 CAPLUS
DN 136:402117
TI Alkoxy-Substituted Poly(p-phenylene 1,3,4-oxadiazole)s: Synthesis,
Chemical Characterization, and Electro-Optical Properties
AU Gillo, M.; Iannelli, P.; Laurienzo, P.; Malinconico, M.; Roviello, A.;
Mormile, P.; Petti, L.
CS Istituto di Chimica e Tecnologia dei Polimeri(ICTP)-CNR, Pozzuoli, Naples,
34-80078, Italy
SO Chemistry of Materials (2002), 14(4), 1539-1547

CODEN: CMATEX; ISSN: 0897-4756
PB American Chemical Society
DT Journal
LA English
AB The synthesis of a series of conjugated aromatic polyoxadiazoles (PODn) characterized by having moderate chain flexibility and highly flexible lateral substituents is reported. The majority of these polymers are soluble in a mixture of chloroform and trifluoroacetic acid and have inherent viscosities up to 0.9 dL/g. The glass transition temperature, Tg, lies in the range 165-230 °C and depends on the side-chain length. The PODn show a good thermal stability in nitrogen up to 270°C. Wide-angle X-ray diffractograms reveal a "comblike" organization of the polymeric chains. Homogeneous thin films of such a material were prepared by the spin-coating technique. Films spun on fused silica were characterized by spectroscopic anal. in the whole UV-vis-NIR range showing a high transmission in the NIR region which is the typical telecommunication band (1300-1500 nm). Furthermore, the refractive index and the film thickness have been measured using the coupled modes technique in a planar guiding structure having POD as the core. A device was prepared consisting of the said polymer sandwiched between two electrodes on top of a glass substrate. The electron conductivity of the polymer has been found to be higher than that of terephthalic poly(1,3,4-oxadiazole).
IT 428516-42-1P 428516-43-2P 428516-44-3P
428516-45-4P
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(synthesis, chemical characterization, and electro-optical properties of alkoxy-substituted poly(p-phenylene-1,3,4-oxadiazoles))
RN 428516-42-1 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-ethoxy-, dihydrazide, polymer with 2-ethoxy-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

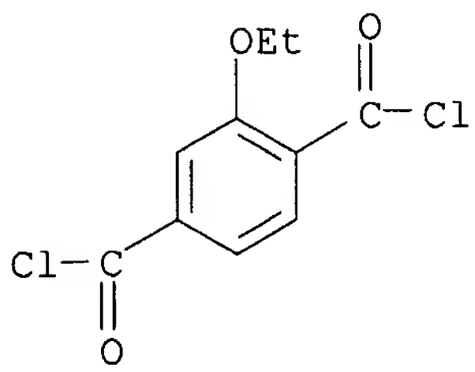
CM 1

CRN 428516-38-5
CMF C10 H14 N4 O3



CM 2

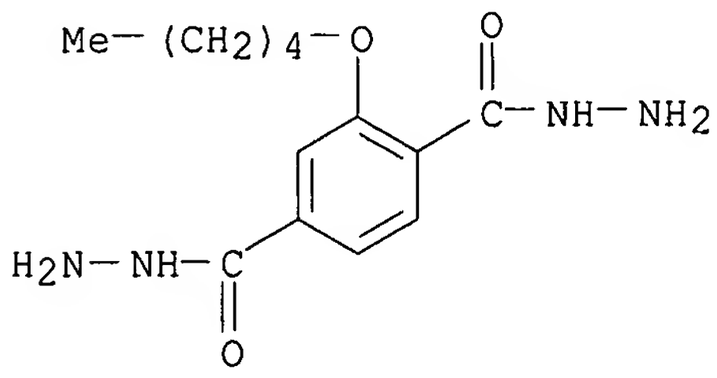
CRN 321588-61-8
CMF C10 H8 Cl2 O3



RN 428516-43-2 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(pentyloxy)-, dihydrazide, polymer with 2-(pentyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

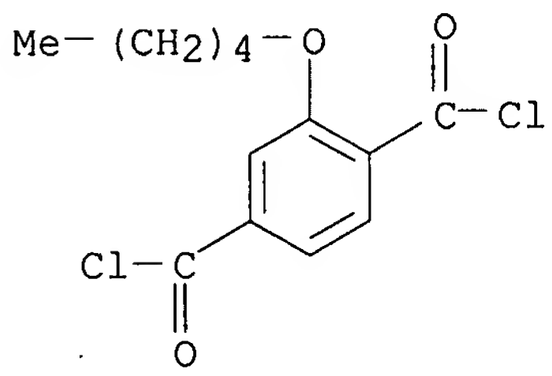
CM 1

CRN 428516-39-6
CMF C13 H20 N4 O3



CM 2

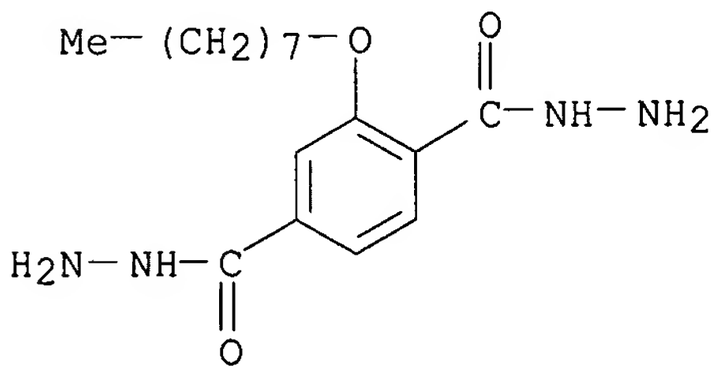
CRN 193150-89-9
CMF C13 H14 Cl2 O3



RN 428516-44-3 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide, polymer with 2-(octyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

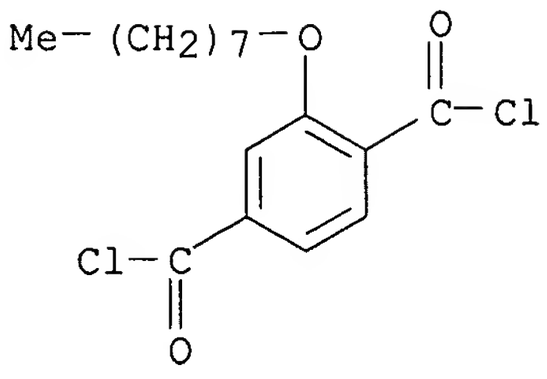
CM 1

CRN 428516-40-9
CMF C16 H26 N4 O3



CM 2

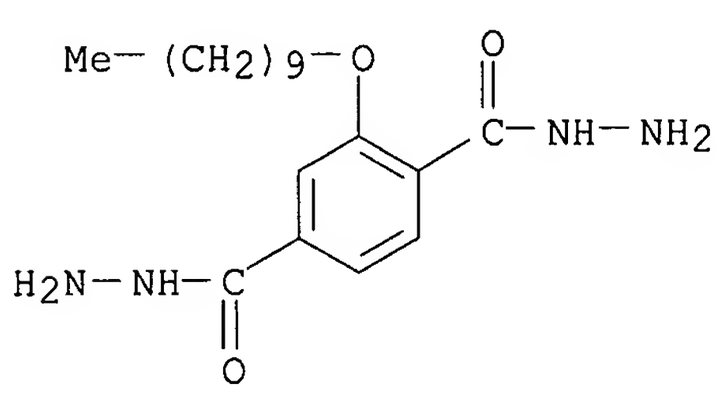
CRN 321588-70-9
CMF C16 H20 Cl2 O3



RN 428516-45-4 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(decyloxy)-, dihydrazide, polymer with 2-(decyloxy)-1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

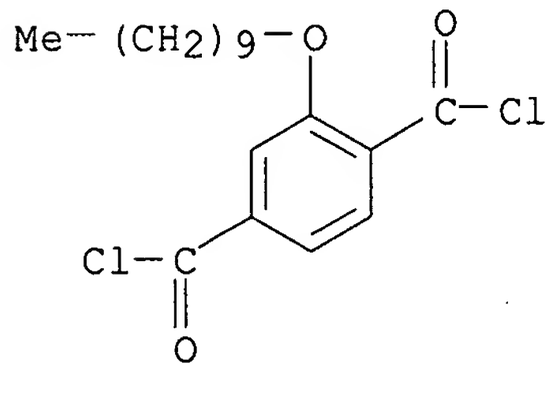
CM 1

CRN 428516-41-0
CMF C18 H30 N4 O3

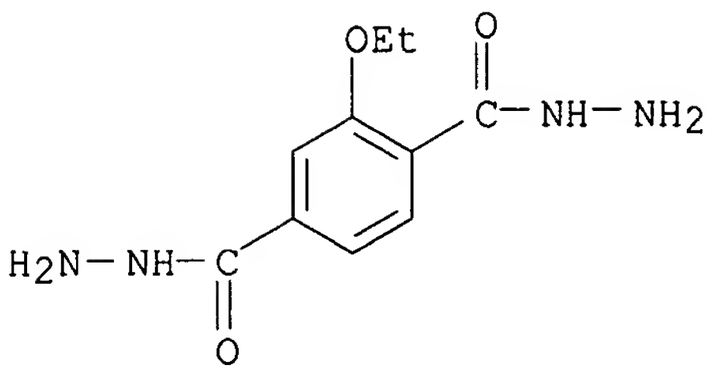


CM 2

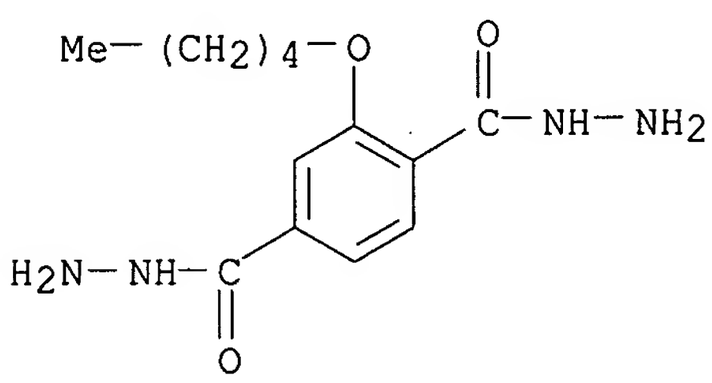
CRN 321588-74-3
CMF C18 H24 Cl2 O3



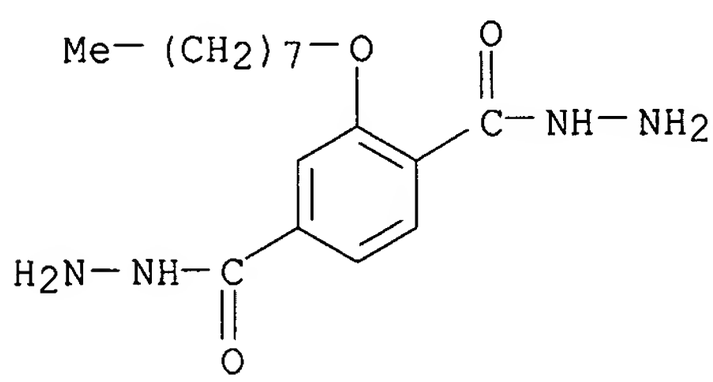
IT 428516-38-5P 428516-39-6P 428516-40-9P
428516-41-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis, chemical characterization, and electro-optical properties of alkoxy-substituted poly(p-phenylene-1,3,4-oxadiazoles))
RN 428516-38-5 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-ethoxy-, dihydrazide (9CI) (CA INDEX NAME)



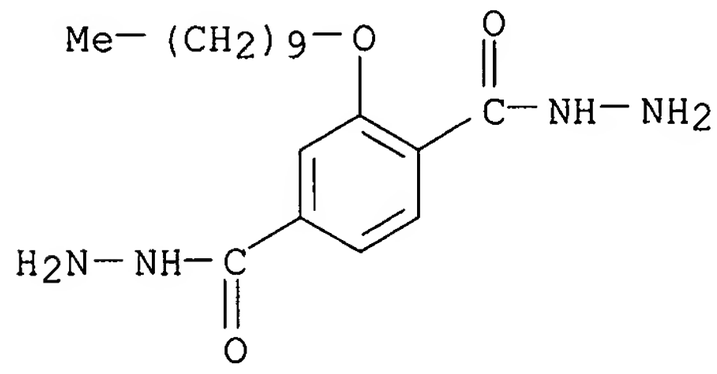
RN 428516-39-6 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(pentyloxy)-, dihydrazide (9CI) (CA INDEX NAME)



RN 428516-40-9 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(octyloxy)-, dihydrazide (9CI) (CA INDEX NAME)



RN 428516-41-0 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2-(decyloxy)-, dihydrazide (9CI) (CA INDEX NAME)



RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:10469 CAPLUS
DN 136:85750
TI Preparation of novel compounds possessing antibacterial, antifungal or antitumor activity
IN Zhang, Wentao; Liehr, Sebastian Johannes R.; Velligan, Mark Douglas;

Dyatkina, Natalia B.; Botyanszki, Janos; Shi, Dong-Fang; Roberts, Christopher Don; Khorlin, Alexander; Nelson, Peter Harold; Muchowski, Joseph Martin

PA Genelabs Technologies, Inc., USA

SO PCT Int. Appl., 141 pp.
CODEN: PIXXD2

DT Patent

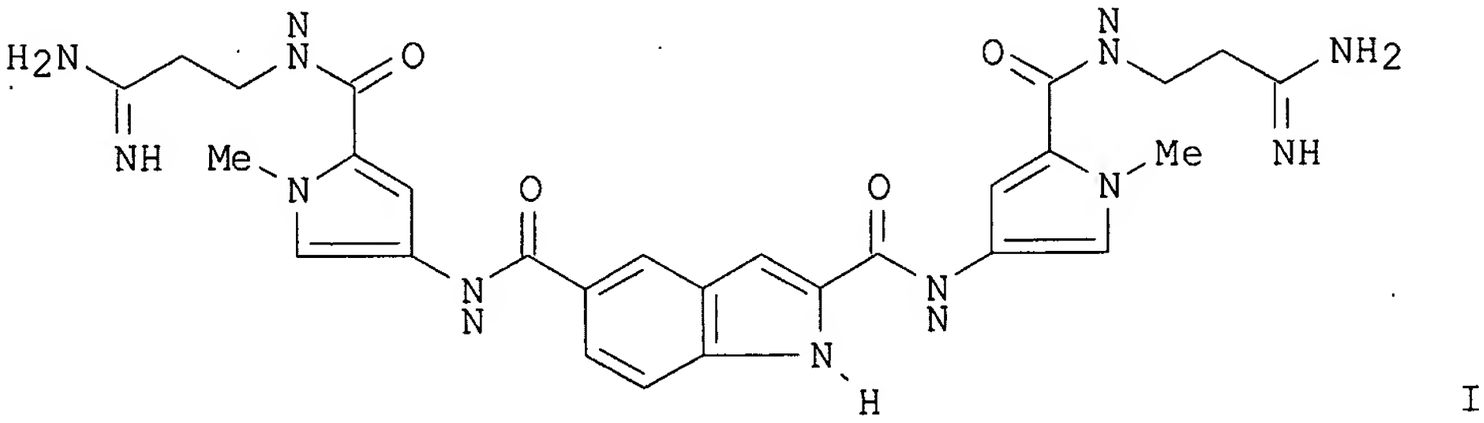
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002000650	A2	20020103	WO 2001-US20334	20010626
	WO 2002000650	A3	20021024		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2414512	A1	20020103	CA 2001-2414512	20010626
	US 2002037856	A1	20020328	US 2001-892327	20010626
	US 6849713	B2	20050201		
	EP 1294713	A2	20030326	EP 2001-948740	20010626
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	BR 2001012030	A	20030429	BR 2001-12030	20010626
	JP 2004501915	T	20040122	JP 2002-505774	20010626
	NZ 522839	A	20041126	NZ 2001-522839	20010626
	US 2003119749	A1	20030626	US 2002-277666	20021023
	US 6906103	B2	20050614		
	NO 2002005720	A	20030226	NO 2002-5720	20021128
	ZA 2002009774	A	20040302	ZA 2002-9774	20021202
	MX 2002PA12271	A	20040906	MX 2002-PA12271	20021211
PRAI	US 2000-214478P	P	20000627		
	US 2001-892327	A3	20010626		
	WO 2001-US20334	W	20010626		

OS MARPAT 136:85750

GI



I

AB Compds. of formula R1Z1COX1NHCOX2CONHX3COZ2R2 (Z1 and Z2 = independently NR3, O; R3 = H, alkyl; R1 and R2 = independently substituted alkyl or aryl,(un)substituted heteroaryl; X2 = (un)substituted aryl or heteroaryl, alkenyl, alkynyl, cycloalkyl, heterocyclic; X1 and X3 = independently (un)substituted aryl or heteroaryl, CHR4; R4 = (un)natural amino acid side chain) or their pharmaceutically acceptable salts were prepared and possess one or more of the following activities: antibacterial, antifungal and antitumor activity. For example, 1H-Indole-2,5-dicarboxylic acid

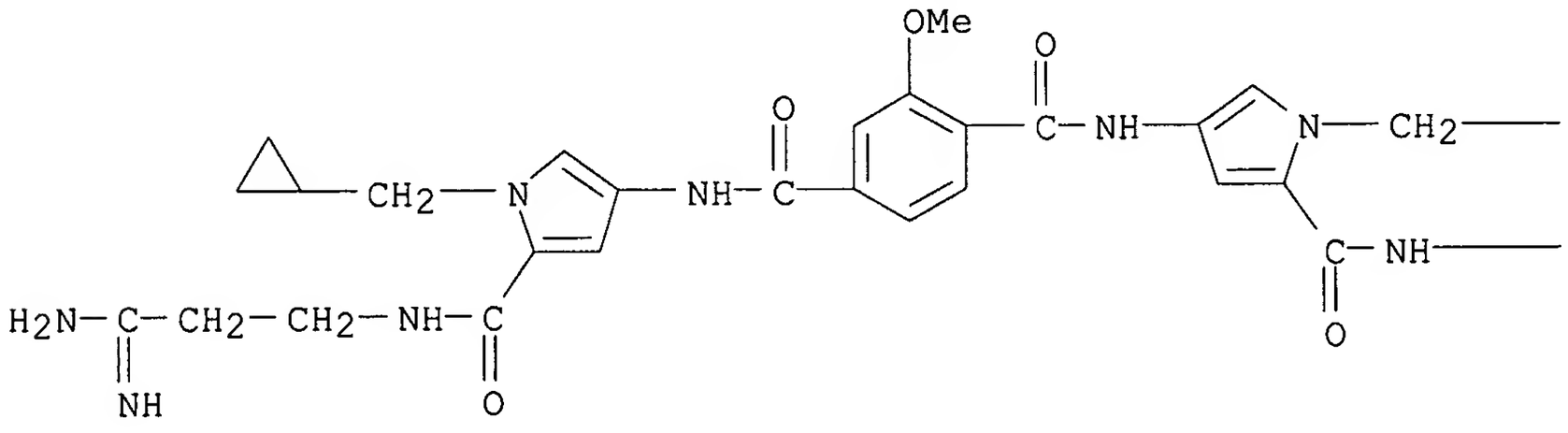
dipentafluorophenyl ester was reacted with at least two equivalent of 4-amino-1-methyl-1H-pyrrole-2-carboxylic acid (2-carbamimidoyl-ethyl)-amide in DMF to give compound I. Compds. of this invention exhibited antibacterial and antifungal activity with some having minimal inhibitory concns. of <45.5 μM. Studies of their DNA binding properties demonstrated that they bind to DNA very tightly, with apparent Kd,app values below 100 nM for most compds. tested.

IT 386253-05-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel compds. possessing antibacterial, antifungal or antitumor activity)

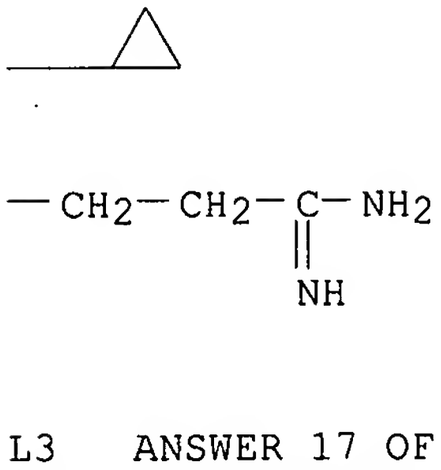
RN 386253-05-0 CAPLUS

CN 1,4-Benzenedicarboxamide, N,N'-bis[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-(cyclopropylmethyl)-1H-pyrrol-3-yl]-2-methoxy- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L3 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2001:403466 CAPLUS
DN 135:24726
TI Polymerizable compositions containing aromatic amide group-containing (meth)acrylic monomers and dental restorative materials
IN Yamakawa, Junichiro; Kazama, Hideki
PA Tokuyama Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001151808	A	20010605	JP 1999-335874	19991126
PRAI	JP 1999-335874		19991126		

AB The compns., which show high fracture toughness and can be substitutes for

metal materials, comprise (A) monomers containing R1(CONHR2COCR3:CH2)n [R1 = mono-, di-, or trivalent C6-24 organic group having 1-3 aromatic ring selected from benzene, naphthalene, and anthracene; R2 = (CB1B2)kA1, (CB1B2)kA1COR4[(CH2)lA2]m, (CB1B2)kA1COR4A2, (CB1B2)kA1COR4CO[(CH2)lA2]m, (CB1B2)kA1[(CH2)lA2]m (A1, A2 = O, NH; B1, B2 = H, C1-5 alkyl, C1-5 alkoxy, Ph; R4 = C1-12 hydrocarbylene; k, l, m = 1-5)], (B) fillers containing 40-99% approx. spherical inorg. particles having average particle size 0.1-5 μm and 1-60% inorg. particles having average particle size 0.01-0.1 μm, and (C) polymerization initiators. The compns. may addnl. contain 10-300 parts [based on 100 parts (B)] amorphous inorg. particles which have average particle size 0.1-9 μm and contain ≤3% those having particle size ≥10 μm. Dental restorative materials comprising the composition are also claimed. A composition containing 1,3-C6H4(CONHCH2CH2OCOC6H4CO2CH2CH2OCOC Me:CH2-3)2 (I) 60, triethylene glycol dimethacrylate 40, 60:40 mixture of spherical SiO2-ZrO2 filler (average particle size 0.52 μm) and spherical SiO2-TiO2 filler (average particle size 0.08 μm) 400, and bis(2,4,6-trimethylbenzoyl)phenylphosphine oxide 0.05 part was irradiated with light and heated at 100° for 20 min to give a cured sample. Fracture toughness of the cured sample 24 h after soaking in H2O at 37° was 3.3 MPa.m1/2, vs. 2.3 MPa.m1/2 for a control prepared from a composition containing Bis-GMA instead of I.

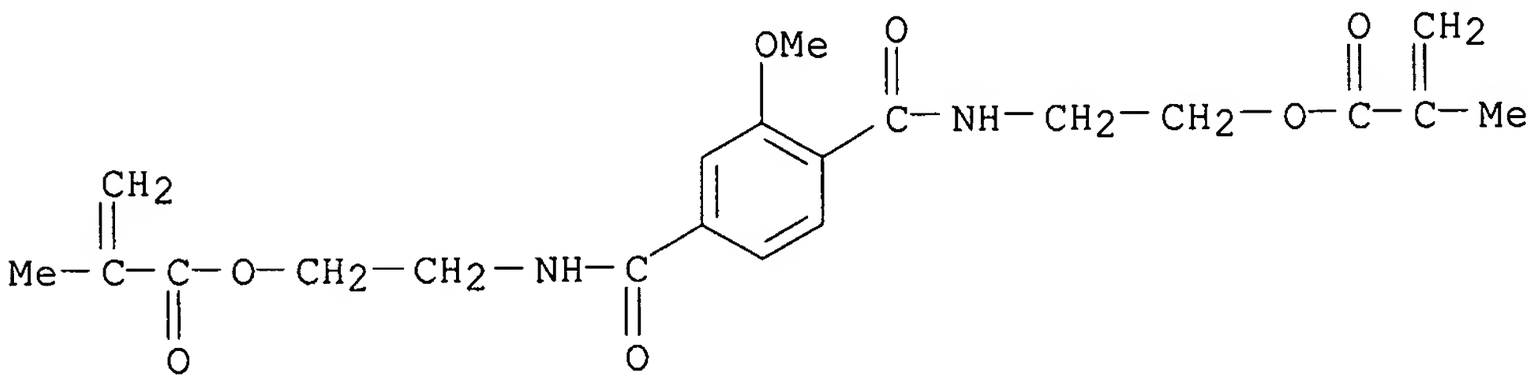
IT 342902-75-4P
RL: PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(polymerizable dental composite resin compns. containing aromatic amide group-containing (meth)acrylic monomers for high fracture strength)

RN 342902-75-4 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester, polymer with (2-methoxy-1,4-phenylene)bis(carbonylimino-2,1-ethanediyl) bis(2-methyl-2-propenoate) (9CI) (CA INDEX NAME)

CM 1

CRN 342902-74-3
CMF C21 H26 N2 O7



CM 2

CRN 109-16-0
CMF C14 H22 O6